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METHODS OF IDENTIFYING MODULATORS OF BROMODOMAINS

FIELD OF THE INVENTION

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The present invention provides the three-dimensional structure of a histone acetyltransferase bromodomain. The three-dimensional structural information is included in the invention. The present invention also identifies for the first time, that bromodomains can bind to an acetylated binding partners. The interaction between bromodomains and their binding partners play a crucial role in various cellular functions, including in the regulation/modulation of DNA transcription. Therefore, the present invention provides procedures for identifying agents that can modulate the interaction of bromodomains and their binding partners by high throughput drug screening and/or through the use of rational drug design based on the three-dimensional data provided herein.

BACKGROUND OF THE INVENTION

In recent years great strides have been made in the elucidation of the steps involved in 20 intercellular and intracellular signaling. Indeed, the individual steps of the cascade of events involved in a number of cellular signal transduction processes have been determined. For example, intercellular signal transduction generally begins with an intercellular ligand binding the extracellular portion of a receptor of the plasma membrane. The bound receptor then either directly or indirectly initiates the activation of one or more cellular factors. An activated cellular factor may act as 25 transcription factor by entering the nucleus to interact with its corresponding genomic response element, or alternatively, it may interact with other cellular factors depending on the complexity of the process. In either case, one or more transcription factors ultimately bind to one or more specific genomic response elements. This 30 binding plays a crucial role in the up and/or down regulation of the transcription of the specific genes that are under the control of these genomic response elements. However, the process of re-organizing the chromatin of eukaryotic cells, which is a prerequisite for the binding of the transcription factor to the genomic response elements, has remained a mystery.

Chromatin contains several highly conserved histone proteins including: H3, H4, H2A, H2B, and H1. These histone proteins package eukaryotic DNA into repeating nucleosomal units that are folded into higher-order chromatin fibers [Luger and Richmond, Curr. Opin. Genet. Dev. 8:140-146 (1998)]. A portion of the histone that comprises roughly a quarter of the protein protrudes from the chromatin surface, and is thereby sensitive to proteolytic enzymes [van Holde, in Chromatin (Rich, A,. ed., Springer, New York) pages111-148 (1988); Hect et al., Cell 80:583-592 (1995)]. This portion of the histone is known as the "histone tail". Histone tails tend to be free for protein-protein interaction, and are also the portion of the histone most prone to post-translational modification. Such post-translational modification includes acetylation, phosphorylation, methylation, ubiquitination, and ADP-ribosylation [van Holde, in Chromatin (Rich, A,. ed., Springer, New York) pages111-148 (1988)].

Of all classes of proteins, histones are amongst the most susceptible to posttranslational modification. Perhaps the best studied post-translational modification of
histones is the acetylation of specific lysine residues [Grunstin, M., Nature, 389:349352 (1997)]. Indeed, acetylation of histone lysine residues has been suggested to
play a pivotal role in chromatin remodeling and gene activation. Consistently,
distinct classes of enzymes, namely histone acetyltransferases (HATs) and histone
deacetylases (HDACs), acetylate or de-acetylate specific histone lysine residues
[Struhl, Genes Dev. 12:599-606 (1998)].

Nearly all known nuclear HATs contain an approximately 110 amino acid sequence
known as the bromodomain [Jeanmougin et al., Trends in Biochemical Sciences,
22:151-153 (1997)], a protein motif that was initially discovered in Drosophila
brahma protein. Bromodomains are found in a large number of chromatin-associated
proteins and have now been identified in approximately 40 proteins, often adjacent to
other protein motifs [Jeanmougin et al., Trends in Biochemical Sciences, 22:151-153
(1997); Tamkun et al., Cell, 68:561-572 (1992): Hanes et al., Nucleic Acids Research,
20:2603 (1992)]. Proteins that contain a bromodomain often contain a second
bromodomain. However, despite the wide occurrence of bromodomains and their

likely role in chromatin regulation, their three-dimensional structure and binding partners heretofore have remained unknown.

Therefore, there is a need to identify a binding partner for a bromodomain. In

addition, there is a need to identify agonists or antagonists to the bromodomainbinding partner complex. Since a preferred method of drug-screening relies on
structure based drug design, there is also a need to determine the three-dimensional
structure of a bromodomain. In this case, once the three dimensional structure of
bromodomain is determined, potential agonists and/or potential antagonists can be

designed with the aid of computer modeling [Bugg et al., Scientific American,
Dec.:92-98 (1993); West et al., TIPS, 16:67-74 (1995); Dunbrack et al., Folding &
Design, 2:27-42 (1997)]. However, heretofore the three-dimensional structure of the
bromodomain has remained unknown. Therefore, there is a need for obtaining a form
of the bromodomain that is amenable for NMR analysis and/or X-ray crystallographic
analysis. Furthermore, there is a need for the determination of the three-dimensional
structure of the bromodomain. Finally, there is a need for procedures for related
structural based drug design predicated on such structural data.

The citation of any reference herein should not be construed as an admission that such reference is available as "Prior Art" to the instant application.

SUMMARY OF THE INVENTION

The present invention provides, for the first time, that bromodomains bind to acetyllysine residues of proteins. The present invention also provides the three-dimensional structure of a bromodomain as well as the three-dimensional structure of a bromodomain-acetyl-histamine complex. The structural information provided can be employed in methods of identifying drugs that can modulate the cellular processes that involve bromodomain-acetyl-lysine interactions. These interactions include chromatin remodeling, which is a required step in eukaryotic transcription. In a particular embodiment, the three-dimensional structural information is used in the design of an inhibitor of leukemia.

The present invention provides an isolated nucleic acid that encodes a peptide consisting of about 21 to 40 amino acids that comprises a ZA loop of a bromodomain. In a preferred embodiment the peptide comprises about 23 to 34 amino acids. The isolated nucleic acid can further comprise a heterologous nucleotide sequence.

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In a preferred embodiment the peptide comprises the amino acid sequence of SEQ ID NO:3. In another embodiment the peptide comprises the amino acid sequence of SEQ ID NO:43. In particular embodiments the ZA loop is obtained from the bromodomain having the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21, or SEQ ID NO: 22, or SEQ ID NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32, or SEQ ID NO:33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36, or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention further provides a recombinant DNA molecule that comprises
an isolated nucleic acid of the present invention, as described above, with or without a
heterologous nucleotide sequence. Such a recombinant DNA molecule can be
operatively linked to an expression control sequence and can be part of an expression
vector. The present invention further provides a cell that comprises such an
expression vector. The cell can be either a eukaryotic or a prokaryotic cell. The
present invention further provides a method of expressing the peptides of the present
invention or fragments thereof in this cell. One such method comprises culturing the
cell in an appropriate cell culture medium under conditions that provide for
expression of the peptide by the cell.

The present invention further provides a peptide consisting of about 21 to 40 amino acids that comprises a ZA loop of a bromodomain. In a preferred embodiment the

peptide comprises about 23 to 34 amino acids. The present invention also provides fusion proteins or peptides comprising these peptides.

In a preferred embodiment the peptide comprises the amino acid sequence of SEQ ID NO:3. In another embodiment the peptide comprises the amino acid sequence of SEQ ID NO:43. In particular embodiments the ZA loop is obtained from the bromodomain having the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21, or SEQ ID NO: 22, or SEQ ID NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32, or SEQ ID NO:33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36, or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO:35, or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention also provides antibodies raised against the peptides/proteins of the present invention, or raised against an antigenic fragment of these proteins/fragments. In a particular embodiment an antibody is raised against a

20 fragment of the ZA loop of a bromodomain. In another embodiment an antibody is raised against a fragment of a protein or peptide that comprises an acetyl-lysine, wherein the protein or peptide can bind to a bromodomain. Such fragments can be conjugated to a carrier protein or be part of a fusion protein. In one embodiment the antibody is a polyclonal antibody. In another embodiment, the antibody is a monoclonal antibody. A hybridoma that makes the monoclonal antibody is also part of the present invention. In a particular embodiment the antibody is a chimeric antibody. Antibodies that can specifically recognize acetyl-lysine residues involved bromodomain binding are also part of the present invention.

In another aspect of the present invention a method is provided for identifying a compound that modulates the affinity of a bromodomain for a ligand (and/or protein) that comprises an acetylated lysine. One such embodiment comprises contacting the

bromodomain and the ligand in the presence of a compound under conditions that, the bromodomain and the ligand bind in the absence of the compound. The affinity of the bromodomain for the ligand is then determined (e.g., measured). A compound is identified as a compound that modulates the affinty of the bromodomain for the ligand when there is a change in the affinity of the bromodomain for the ligand in the presence of the compound. When the affinity of the bromodomain for the ligand increases in the presence of the compound, the compound is identified as a promoting agent for the bromodomain-ligand complex. When the affinity of the bromodomain for the ligand decreases in the presence of the compound, the compound is identified as an inhibitor of the bromodomain-ligand complex. In a preferred embodiment, the compound to be tested is pre-selected by performing rational drug design with the set of atomic coordinates obtained from one or more of Tables 1-6. More preferably the selecting is performed in conjunction with computer modeling. In a particular embodiment, the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the threedimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7 alone or with acetyl-histamine.

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The present invention also provides a method of identifying a compound that modulates the stability of a bromodomain-acetyl-lysine binding complex. One such 20 embodiment comprises contacting the bromodomain-acetyl-lysine binding complex in the presence of the compound under conditions in which the bromodomain-acetyllysine binding complex forms in the absence of the compound. The stability of the bromodomain-acetyl-lysine binding complex is then determined (e.g., measured). A 25 compound is identified as a compound that modulates the stability of the bromodomain-acetyl-lysine binding complex, when there is a change in the stability of the bromodomain-acetyl-lysine binding complex in the presence of that compound. When the stability of the bromodomain-acetyl-lysine binding complex increases in the presence of the compound, the compound is identified as a stabilizing agent. When the stability of the bromodomain-acetyl-lysine binding complex decreases in the 30 presence of the compound, the compound is identified as an inhibitor. In a preferred embodiment, the compound to be tested is pre-selected by performing rational drug

design with the set of atomic coordinates obtained from one or more of Tables 1-6. More preferably the selecting is performed in conjunction with computer modeling. In a particular embodiment, the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the three-dimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7 alone or with acetyl-histamine.

As anyone having skill in the art of drug development would readily understand, the potential drugs selected by the above methodologies can be refined by re-testing in appropriate drug assays, including those disclosed herein. Chemical analogs of such potential drugs can be obtained (either through chemical synthesis or drug libraries) and be analogously tested. Therefore, methods comprising successive iterations of the steps of the individual drug assays, as exemplified herein, using either repetitive or different binding studies, or transcription activation studies or other such studies are envisioned in the present invention. In addition, potential drugs may be identified first by rapid throughput drug screening, as described below, prior to performing computer modeling on a potential drug using the three-dimensional structure of the bromodomain.

The present invention further comprises all of the potential, selected, and putative compounds (drugs) identified by the methods of the present invention, as well as the final drugs themselves identified with the methods of the present invention.

The present invention further provides a method for identifying a potential binding
partner for a protein (e.g., a histone) comprising an acetyl-lysine. One such
embodiment comprises contacting the protein with a polypeptide comprising a
bromodomain. In a preferred embodiment the bromodomain comprises the amino
acid sequence of SEQ ID NO:3. In particular embodiments the bromodomain has the
amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID
NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14,
or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ
ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21, or SEQ ID NO: 22, or SEQ ID

NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32, or SEQ ID NO:33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36, or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention further provides a method for identifying a protein having a bromodomain. One such embodiment comprises contacting a cellular extract with a peptide comprising an acetyl-lysine.

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The present invention further provides agents that can inhibit the binding of a bromodomain with a protein comprising an acetyl-lysine. In one embodiment the agent is ISYGR-AcK-KRRQRR (SEQ ID NO:4). In another embodiment the agent is ARKSTGG-AcK-APRKQL (SEQ ID NO:5). In still another embodiment the agent is QSTSRHK-AcK-LMFKTE (SEQ ID NO:6). In yet another embodiment the agent is an analog of acetyl-lysine such as acetyl-histamine. In still another embodiment the agent is an antibody that recognizes an acetyl-lysine of a protein binding partner of a bromodomain. In a preferred embodiment the agent is an antibody raised against a ZA loop of a bromodomain. These agents can be used as pharmaceuticals in compositions that contain a pharmaceutically acceptable carrier for example, or in the various drug assays of the present invention, serving as controls to demonstrate specificity.

Accordingly, it is a principal object of the present invention to provide the threedimensional coordinates of a bromodomain.

It is a further object of the present invention to provide the three-dimensional coordinates of a bromodomain complexed with acetyl-histamine.

It is a further object of the present invention to provide an assay for identifying proteins that contain bromodomains that bind proteins that comprise acetyl-lysine.

It is a further object of the present invention to provide methods of identifying drugs that can modulate the bromodomain-acetyl-lysine binding complex.

It is a further object of the present invention to provide methods of identifying drugs that can inhibit the binding of a bromodomain to a protein containing acetyl-lysine.

It is a further object of the present invention to provide methods that incorporate the use of rational design for identifying such drugs.

It is a further object of the present invention to provide a method of identifying drugs that can treat leukemia.

It is a further object of the present invention to provide a method of identifying drugs that can treat and/or prevent AIDS.

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These and other aspects of the present invention will be better appreciated by reference to the following drawings and Detailed Description.

BRIEF DESCRIPTION OF THE DRAWINGS

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Figure 1. Structure-based sequence alignment of a selected number of bromodomains. The sequences were aligned based on the NMR-derived structure of the P/CAF bromodomain, and the predicated four α-helices are shown in green boxes.

Bromodomains are grouped on the basis of the sequence and/or functional similarities as described by Jeanmougin *et al.*, [Trends in Biochemical *Sciences*, 22:151-153 (1997)]. Residue numbers of the P/CAF bromodomain are indicated above its sequence. Three absolutely conserved residues, corresponding to Pro751, Pro767, and Asn803 in the P/CAF bromodomain, are shown in red. Highly conserved residues are colored in blue. The residues of the P/CAF bromodomain that interact with acetyl-histamine, as determined by intermolecular NOEs, are indicated by asterisks. The ZA loop, which is critical for acetyl-lysine binding, for each of the indicated bromodomains is also identified. The underlined residues were changed individually

by site-directed mutagenesis to Ala. Genbank accession numbers for the proteins are as indicated in Table 8, in the Example below, along with the SEQ ID NOs. for the bromodomain sequences.

- Figures 2A-2H depict the structure of the P/CAF bromodomain. Figures 2A-2B shows the stereoview of the C_{α} trace of 30 superimposed NMR-derived structures of the bromodomain (residues 722-830). The N-terminal four residues (SKEP) which are structurally disordered are omitted for clarity. For the final 30 structures, the root-mean-square deviations (RMSDs) of the backbone and all heavy atoms are 0.63 10 \pm 0.11Å and 1.15 \pm 0.12Å for residues 723-830, respectively. The RMSDs of the backbone and all heavy atoms for the four α -helices (residues 727-743, 770-776, 785-802, and 807-827), are 0.34 ± 0.04 Å and 0.87 ± 0.06 Å, respectively. Figures 2C-2D show the stereoview of the bromodomain structures from the bottom of the protein, which is rotated approximately 90° from the orientation in Figures 2A-2B. Figure 2E shows the Ribbons [Carson, M., J. Appl. Crystallogr. 24:958-961 (1991)] 15 depiction of the averaged minimized NMR structure of the P/CAF bromodomain. The orientation of Figure 2E is as shown in Figures 2A-2B. Figures 2F-2G are schematic representations of the overall topology of the up-and-down four-helix bundle folds with the opposite handedness. The left-handed fold is seen in 20 bromodomain, cytochrome b_5 , and T4 lysozyme (left, Figure 2F), whereas the right-handed four-helix bundles are observed in proteins such as hemerythrin and cytochrome b₅₆₂ (right, Figure 2G) [Richardson, J., Adv. Protein Chem., 34:167-339 (1989); Presnell and Cohen, Proc. Natl. Acad. Sci. USA 86:6592-6596 (1989)]. Figure 2H is a molecular surface representation of the electrostatic potential (blue = positive; red = negative) of the bromodomain calculated in GRASP [Nicholls et al., 25 Biophys. J. 64:166-170 (1993)]. The hydrophobic and aromatic residues (Tyr809, Tyr802, Tyr760, Ala757, and Val752) located between the ZA and BC loops are
- Figures 3A-3C show the binding of the P/CAF bromodomain to AcK. Figure 3A shows the superimposed region of the 2D ¹⁵N-HSQC spectra of the bromodomain (approximately 0.5 mM) in its free form (red) and complexed to the AcK-containing

indicated.

H4 peptide (molar ratio 1:6) (black). Figure 3B is the Ribbon and dotted-surface diagram of the bromodomain depicting the location of the lysine-acetylated H4 peptide binding site. The color coding reflects the chemical shift changes ($\Delta \delta$) of the backbone amide ¹H and ¹⁵N resonances upon binding to the AcK peptide as observed in the ¹⁵N-HSQC spectra. The normalized weighted average of the chemical shift changes was calculated by $\Delta_a/\Delta_{max} = [\Delta \delta_{NH} + \Delta \delta_N/25)/2]^{1/2}/\Delta_{max}$, where Δ_{max} is the maximum weighted chemical shift difference observed for Tyr809 (0.16ppm). The backbone atoms are color-coded in red, yellow, or green for residues that have Δ_a/Δ_{max} of >0.6 (Tyr809, Glu808, Asn803, and Ala757), 0.2-0.6 (Ala813, Tyr802, Tyr760, and Val752), or <0.2 (Cys812, Ser807, Cys799, Phe796, and Phe748), respectively. The non-perturbed residues are shown in blue. Figure 3C shows the chemical structures of acetyl-lysine, acetyl-histamine, and acetyl-histidine.

Figure 4 depicts the acetyl-lysine binding pocket. This is the Ribbons [Carson, M., J. Appl. Crystallogr. 24:958-961 (1991)] depiction of a portion of the P/CAF bromodomain complexed with the acetyl-histamine. The ligand is color-coded by atom type.

DETAILED DESCRIPTION OF THE INVENTION

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The present invention identifies a general binding partner (ligand) for the protein motif known as the bromodomain. Indeed, by combining structural and site-directed mutagenesis studies the present invention demonstrates that bromodomains can interact specifically with acetyl-lysine (AcK), making them the first protein modules known to exhibit such interactions. Like other modular domains, such as Src homology-2 (SH2) and phosphotyrosine binding (PTB) domains, which specifically interact with phosphotyrosine-containing proteins, the bromodomain/acetyl-lysine recognition provides a means to regulate protein-protein interactions via protein lysine acetylation. The nature of the acetyl-lysine recognition by the bromodomain is similar to that of histone acetyltransferase interaction with acetyl-CoA. The present invention therefore couples for the first time, the functionality of the bromodomain with the HAT activity of coactivators in the regulation of gene transcription.

The present invention further provides both a nuclear magnetic resonance (NMR) structure of the bromodomain from the HAT coactivator P/CAF (p300/CBP-associated factor) as well as the structure for the P/CAF bromodomain in complex with acetyl-histamine. The structure reveals an unusual left-handed up-and-down four-helix bundle.

The results disclosed herein explain prior deletion experiments which showed that the bromodomain is indispensable for the function of GCN5 in yeast.

Bromodomain-AcK binding also appears to be important for the assembly and activity of multiprotein complexes in transcriptional activation. The results reported herein therefore, form the foundation for identifying specific biological ligands and for defining the molecular mechanisms by which the extensive family of bromodomains participate in chromatin remodeling and transcriptional activation

As disclosed herein, the binding partner for the bromodomain is a peptide or protein comprising an acetyl-lysine (AcK). Interestingly, whereas a free acetyl-lysine does not appear to bind the bromodomain, an analog of the acetyl-lysine, acetyl-histamine, does. This is most likely due to the additional charge present in the free amino acid. Consistently, free acetyl-histidine also does not to bind the bromodomain.

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The present invention further provides a key region of the bromodomain for the interaction with its acetyl-lysine binding partner, the ZA loop. The amino acid sequence of the ZA loop is defined in Figure 1 for a number of bromodomains and is depicted in Figure 2A for P/CAF. In a particular embodiment, the ZA loop has between about 21 and 40 amino acid residues comprising the amino acid sequence of:

$$F X_{2-3} P X_{5-8} J_{P/K/H} X Y J_{Y/F/H} X_5 P J_{M/I/V} D$$
 (SEQ ID NO:3)

more preferably the ZA loop has about 23 to 34 amino acid residues and comprises the amino acid sequence:

$$X_2 F X_{2-3} P X_{5-8} J_{P/K/H} X Y J_{V/F/H} X_5 P J_{M/I/V} D$$
 (SEQ ID NO:43)

- (1) The single letter amino acid code is used in this description, *i.e.*, "F" for phenylalanine; "P" for proline; "Y" for tyrosine; and "D" for aspartic acid.
- (2) "X" indicates any amino acid (an undesignated amino acid); and X, X_2 , X_{2-3} , X_5 , and X_{5-8} indicates one undesignated amino acid, two consecutive undesignated amino acids, two or three consecutive undesignated amino acids, five consecutive undesignated amino acids, and five to eight consecutive undesignated amino acids respectively.
- (3) "J" indicates that identity of the amino acid is restricted to a particular group, again the one letter code is used
 - (i) $J_{P/K/H}$ is either proline, lysine or histidine.
 - (ii) $J_{Y/F/H}$ is either tyrosine, phenylalanine or histidine.
 - (iii) $J_{M/N}$ is either methionine, isoleucine, or valine.

Since this region of the bromodomain is important in binding its acetyl-lysine binding partner, antibodies specifically raised against this region are also included in the present invention. In a particular embodiment, the antibody is a humanized chimeric antibody that can be used in therapeutic treatment. Thus monoclonal, chimeric, and polyclonal antibodies raised against bromodomains, preferably against amino acid residues in the ZA loop region are part of the present invention. In a specific embodiment the antibody is raised against a peptide, fusion peptide or conjugated peptide consisting of amino acid residues 746 to 765 of SEQ ID NO:2, *i.e.*, WPFMEPVKRTEAPGYYEVIR (SEQ ID NO:44). Such antibodies can be used in the treatment of leukemia for example. Alternatively, these antibodies can be used in drug discovery assays.

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Thus the present invention provides the first detailed structural information regarding a bromodomain and a bromodomain complexed with its acetylated binding partner. The present invention therefore provides the three-dimensional structure of the bromodomain and a bromodomain acetylated binding partner complex. Since the interaction of the bromodomain with a histone for example, can play a significant role in chromatin remodeling/regulation, the structural information provided herein can be employed in methods of identifying drugs that can modulate basic cell processes by modulating the transcription. In a particular embodiment, the three-dimensional

structural information is used in the design of a small organic molecule for the treatment of cancer.

Indeed, the bromodomain and lysine-acetylated protein interaction can now be implicated to play a causal role in the development of a number of diseases including cancers such as leukemia. For example, chromatin remodeling plays a central role in the etiology of viral infection and cancer [Archer and Hodin, Curr. Opin, Genet. Biol. 9:171-174 (1999); Jacobson and Pillus, Curr. Opin. Genet. Biol. 9:175-184 (1999)]. Both altered histone acetylation/deacetylation and aberrant forms of chromatin-10 remodeling complexes are associated with human diseases. Furthermore, chromosomal translocation of various cellular genes with those encoding HATs and subunits of chromatin remodeling complexes have been implicated in leukomogenesis. The MOZ (monocytic leukemia zinc finger) and MLL/ALL-1 genes are frequently fused to the gene encoding the co-activator HAT CBP [Sobulo et al., Proc. Natl. Acad. Sci. 15 USA 94:8732-8737(1997)]. The resulting fusion protein MLL-CBP contains the tandem bromodomain-PHD finger-HAT domain of CBP. It also has been shown that both the bromodomain and HAT domain of CBP are required for leukomogenesis, because deletion of either the bromodomain or the HAT domain results in loss of the MLL-CBP fusion protein's ability for cell transform. These results indicate that the 20 CBP bromodomain, and more particularly, the ZA loop of the CBP bromodomain, is an excellent target for developing drugs that interfere with the bromodomain acetyllysine interaction that can be used in the treatment of human acute leukemia. In addition, an antibody (e.g., a humanized antibody) raised specifically against a peptide from the ZA loop of the CBP bromodomain could also be effective for treating these 25 conditions.

Furthermore, the human immunodeficiency virus type 1 (HIV-1) trans-activator protein, Tat, is absolutely required for productive HIV viral replication [Jeang and Gatignol, Curr. Top. Microbiol. Immunol., 188:123-144(1994)]. Recently, it has been shown that HIV-1 Tat transcriptional activity is tightly regulated by lysine acetylation [Kiernan et al., EMBO Journal 18:6106-6118 (1999)]. Therefore, the interaction of the acetyl-lysine of Tat with one or more bromodomain-containing proteins associated

with chromatin remodeling could mediate gene transcription. Thus, the bromodomain/lysine-acetylated Tat interaction could also serve as a drug target for blocking HIV replication in cells. Similarly, an antibody raised specifically against a peptide from the ZA loop of the bromodomain could also be effective for treating these conditions.

In addition, based on the new structural information disclosed herein, the key amino acid residues for the binding of a given bromodomain and its binding partner can be identified and further elucidated using basic mutagenesis and standard isothermal titration calorimetry, for example. In this case, both the crucial amino acids for the bromodomain and the binding partner (i.e., apart from the acetyl-lysine) can be readily determined and are also part of the present invention.

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The results obtained from the structural and functional studies disclosed herein provide
the foundation for both high throughput drug screening and structure-based rational
drug design. The agents identified by this procedure will be useful for ameliorating
conditions involving chromatin remodeling/regulation as indicated above.

Structure based rational drug design is the most efficient method of drug development.

However, heretofore, no information has been disclosed regarding the structure of the bromodomain or more importantly, its interaction with the acetyl-lysine of its binding partner. Obtaining detailed structural information requires an extensive NMR or X-ray crystallographic analysis. By determining and then exploiting the detailed structural information of the bromodomain and of the bromodomain/acetyl-histamine

(exemplified by NMR analysis below) the present invention provides novel methods for developing new drugs through structure based rational drug design.

Thus the present invention provides representative sets of the atomic structure coordinates of the free form of the P/CAF bromodomain (Table 5) and of the P/CAF bromodomain-acetyl-histamine complex (Table 6) which were both obtained by NMR analysis. A Ribbon diagram of the three-dimensional structure of the P/CAF bromodomain is depicted in Figure 2E, whereas the P/CAF bromodomain acetyl-lysine

binding pocket is depicted in Figure 4. The present invention also provides the NOE-derived distance restraints, and NMR chemical shift assignments of the P/CAF bromodomain. The NMR chemical shift assignments of the P/CAF bromodomain are included in the chemical shift table (Table 1) for the ¹H-¹⁵N HSQC spectrum of P/CAF bromodomain. The unambiguous NOE-derived Inter-proton Distance Restraints (Table 2), the ambiguous NOE-derived Inter-proton Distance Restraints (Table 3) and the ¹H bonding restraints (Table 4) are also disclosed herein. The sample atomic coordinate data provided enable the skilled artisan to practice the invention. In addition, Tables 1-6 are also capable of being placed into a computer readable form which is also part of the present invention. Furthermore, methods of using these coordinates and chemical shifts and related information (including in computer readable forms) either individually or together in drug assays are also provided. More particularly, such atomic coordinates can be used to identify potential ligands or drugs which will modulate the binding of a bromodomain with its binding partner.

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Therefore, if appearing herein, the following terms shall have the definitions set out below.

As used herein a "bromodomain-acetyl-lysine binding complex" is a binding complex between a bromodomain or fragment thereof and either a peptide/polypeptide comprising an acetyl-lysine (or an analog of acetyl-lysine), or a free analog of acetyl-lysine, such as acetyl-histamine disclosed in the Example below. Preferably, the peptide comprises at least six amino acids in addition to the acetyl-lysine. The dissociation constant of a bromodomain-acetyl-lysine binding complex is dependent on whether the lysine residue or analog thereof is acetylated or not, such that the affinity for the bromodomain and the peptide comprising the lysine residue (for example) significantly decreases when that lysine residue is not acetylated.

As used herein a "ZA loop" of a bromodomain is one protion of a bromodomain that is involved in the binding of the bromodomain to the acetyl-lysine. The structure of the ZA loop of the bromodomain of for P/CAF is depicted in Figure 2A. The ZA loop has between about 20 and 40 amino acids and comprises the amino acid sequence of SEQ ID NO:3. More preferably the ZA loop comprises between about 23 to 34 amino acids

and has the amino acid sequence SEQ ID NO:43. The amino acid sequence of the ZA loop for a representative number of individual bromodomains is shown in Figure 1.

A "polypeptide" or "peptide" comprising a fragment of a bromodomain, such as the ZA loop, or a peptide or polypeptide comprising an acetyl-lysine, as used herein can be the "fragment" alone, or a larger chimeric or fusion peptide/protein which contains the "fragment".

As used herein the terms "fusion protein" and "fusion peptide" are used interchangeably and encompass "chimeric proteins and/or chimeric peptides" and fusion "intein proteins/peptides". A fusion protein comprises at least a portion of a protein or peptide of the present invention, e.g., a bromodomain, joined via a peptide bond to at least a portion of another protein or peptide including e.g., a second bromodomain in a chimeric fusion protein. In a particular embodiment the portion of the bromodomain is antigenic. Fusion proteins can comprise a marker protein or peptide, or a protein or peptide that aids in the isolation and/or purification of the protein, for example.

As used herein, and unless otherwise specified, the terms "agent", "potential drug", "compound", "test compound" or "potential compound" are used interchangeably, and refer to chemicals which potentially have a use as an inhibitor or activator/stabilizer of bromodomain-acetyl-lysine binding. Therefore, such "agents", "potential drugs", "compounds" and "potential compounds" may be used, as described herein, in drug assays and drug screens and the like.

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As used herein a "small organic molecule" is an organic compound, including a peptide [or organic compound complexed with an inorganic compound (e.g., metal)] that has a molecular weight of less than 3 Kilodaltons. Such small organic molecules can be included as agents, etc. as defined above.

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As used herein the term "binds to" is meant to include all such specific interactions that result in two or more molecules showing a preference for one another relative to some third molecule. This includes processes such as covalent, ionic, hydrophobic and

hydrogen bonding but does not include non-specific associations such as solvent preferences.

As used herein the term "about" signifies that a value is within twenty percent of the indicated value *i.e.*, a peptide containing "about" 20 amino acid residues can contain between 16 and 24 amino acid residues.

General Techniques for Constructing Nucleic Acids That Encode the Bromodomains and Fragments Thereof (Incuding, ZA Loops); and the Bromodomain Binding Partners of the Present Invention.

In accordance with the present invention there may be employed conventional molecular biology, microbiology, and recombinant DNA techniques within the skill of the art. Such techniques are explained fully in the literature. See, e.g., Sambrook,

- 15 Fritsch & Maniatis, Molecular Cloning: A Laboratory Manual, Second Edition (1989)
 Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York (herein
 "Sambrook et al., 1989"); DNA Cloning: A Practical Approach, Volumes I and II
 (D.N. Glover ed. 1985); Oligonucleotide Synthesis (M.J. Gait ed. 1984); Nucleic Acid
 Hybridization [B.D. Hames & S.J. Higgins eds. (1985)]; Transcription And
- 20 Translation [B.D. Hames & S.J. Higgins, eds. (1984)]; Animal Cell Culture [R.I. Freshney, ed. (1986)]; Immobilized Cells And Enzymes [IRL Press, (1986)]; B. Perbal, A Practical Guide To Molecular Cloning (1984); F.M. Ausubel et al. (eds.), Current Protocols in Molecular Biology, John Wiley & Sons, Inc. (1994).
- Therefore, if appearing herein, the following terms shall have the definitions set out below.

As used herein, the term "gene" refers to an assembly of nucleotides that encode a polypeptide, and includes cDNA and genomic DNA nucleic acids.

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A "vector" is a replicon, such as plasmid, phage or cosmid, to which another DNA segment may be attached so as to bring about the replication of the attached segment. A "replicon" is any genetic element (e.g., plasmid, chromosome, virus) that functions

as an autonomous unit of DNA replication in vivo, i.e., capable of replication under its own control.

A "cassette" refers to a segment of DNA that can be inserted into a vector at specific restriction sites. The segment of DNA encodes a polypeptide of interest, and the cassette and restriction sites are designed to ensure insertion of the cassette in the proper reading frame for transcription and translation.

A cell has been "transfected" by exogenous or heterologous DNA when such DNA has been introduced inside the cell.

A "nucleic acid molecule" refers to the phosphate ester polymeric form of ribonucleosides (adenosine, guanosine, uridine or cytidine; "RNA molecules") or deoxyribonucleosides (deoxyadenosine, deoxyguanosine, deoxythymidine, or deoxycytidine; "DNA molecules"), or any phosphoester analogues thereof, such as phosphorothioates and thioesters, in either single stranded form, or a double-stranded helix. Double stranded DNA-DNA, DNA-RNA and RNA-RNA helices are possible. The term nucleic acid molecule, and in particular DNA or RNA molecule, refers only to the primary and secondary structure of the molecule, and does not limit it to any particular tertiary forms. Thus, this term includes double-stranded DNA found, inter alia, in linear or circular DNA molecules (e.g., restriction fragments), plasmids, and chromosomes. In discussing the structure of particular double-stranded DNA molecules, sequences may be described herein according to the normal convention of giving only the sequence in the 5' to 3' direction along the nontranscribed strand of 25 DNA (i.e., the strand having a sequence homologous to the mRNA). A "recombinant DNA molecule" is a DNA molecule that has undergone a molecular biological manipulation.

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A nucleic acid molecule is "hybridizable" to another nucleic acid molecule, such as a cDNA, genomic DNA, or RNA, when a single stranded form of the nucleic acid molecule can anneal to the other nucleic acid molecule under the appropriate conditions of temperature and solution ionic strength (see Sambrook et al., supra). The conditions of temperature and ionic strength determine the "stringency" of the

hybridization. For preliminary screening for homologous nucleic acids, low stringency hybridization conditions, corresponding to a T_m of 55°, can be used, e.g., 5x SSC, 0.1% SDS, 0.25% milk, and no formamide; or 30% formamide, 5x SSC, 0.5% SDS). Moderate stringency hybridization conditions correspond to a higher T_m, e.g., 40% formamide, with 5x or 6x SCC. High stringency hybridization conditions correspond to the highest T_m, e.g., 50% formamide, 5x or 6x SCC. Hybridization requires that the two nucleic acids contain complementary sequences, although depending on the stringency of the hybridization, mismatches between bases are possible. The appropriate stringency for hybridizing nucleic acids depends on the length of the 10 nucleic acids and the degree of complementation, variables well known in the art. The greater the degree of similarity or homology between two nucleotide sequences, the greater the value of T_m for hybrids of nucleic acids having those sequences. The relative stability (corresponding to higher T_m) of nucleic acid hybridizations decreases in the following order: RNA:RNA, DNA:RNA, DNA:DNA. For hybrids of greater 15 than 100 nucleotides in length, equations for calculating T_m have been derived (see Sambrook et al., supra, 9.50-10.51). For hybridization with shorter nucleic acids, i.e., oligonucleotides, the position of mismatches becomes more important, and the length of the oligonucleotide determines its specificity (see Sambrook et al., supra, 11.7-11.8). Preferably a minimum length for a hybridizable nucleic acid is at least about 12 20 nucleotides; preferably at least about 18 nucleotides; and more preferably the length is at least about 27 nucleotides; and most preferably 36 nucleotides.

In a specific embodiment, the term "standard hybridization conditions" refers to a T_m of 55°C, and utilizes conditions as set forth above. In a preferred embodiment, the T_m is 60°C; in a more preferred embodiment, the T_m is 65°C.

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A DNA "coding sequence" is a double-stranded DNA sequence which is transcribed and translated into a polypeptide in a cell *in vitro* or *in vivo* when placed under the control of appropriate regulatory sequences. The boundaries of the coding sequence are determined by a start codon at the 5' (amino) terminus and a translation stop codon at the 3' (carboxyl) terminus. A coding sequence can include, but is not limited to, prokaryotic sequences and synthetic DNA sequences. If the coding sequence is

intended for expression in a eukaryotic cell, a polyadenylation signal and transcription termination sequence will usually be located 3' to the coding sequence.

Transcriptional and translational control sequences are DNA regulatory sequences, such as promoters, enhancers, terminators, and the like, that provide for the expression of a coding sequence in a host cell. In eukaryotic cells, polyadenylation signals are control sequences.

A "promoter sequence" is a DNA regulatory region capable of binding RNA

10 polymerase in a cell and initiating transcription of a downstream (3' direction) coding sequence. For purposes of defining the present invention, the promoter sequence is bounded at its 3' terminus by the transcription initiation site and extends upstream (5' direction) to include the minimum number of bases or elements necessary to initiate transcription at levels detectable above background. Within the promoter sequence

15 will be found a transcription initiation site (conveniently defined for example, by mapping with nuclease S1), as well as protein binding domains (consensus sequences) responsible for the binding of RNA polymerase.

A coding sequence is "under the control" of transcriptional and translational control sequences in a cell when RNA polymerase transcribes the coding sequence into mRNA, which is then trans-RNA spliced and translated into the protein encoded by the coding sequence.

A DNA sequence is "operatively linked" to an expression control sequence when the
expression control sequence controls and regulates the transcription and translation of
that DNA sequence. The term "operatively linked" includes having an appropriate
start signal (e.g., ATG) in front of the DNA sequence to be expressed and maintaining
the correct reading frame to permit expression of the DNA sequence under the control
of the expression control sequence and production of the desired product encoded by
the DNA sequence. If a gene that one desires to insert into a recombinant DNA
molecule does not contain an appropriate start signal, such a start signal can be inserted
in front of the gene.

As used herein, the term "homologous" in all its grammatical forms refers to the relationship between proteins that possess a "common evolutionary origin," including proteins from superfamilies (e.g., the immunoglobulin superfamily) and homologous proteins from different species (e.g., myosin light chain, etc.) [Reeck et al., Cell, 50:667 (1987)]. Such proteins have sequence homology as reflected by their high degree of sequence similarity.

Accordingly, the term "sequence similarity" in all its grammatical forms refers to the degree of identity or correspondence between nucleic acid or amino acid sequences of proteins that may or may not share a common evolutionary origin (see Reeck et al., supra). However, in common usage and in the instant application, the term "homologous," when modified with an adverb such as "highly," may refer to sequence similarity and not a common evolutionary origin.

15 Two DNA sequences are "substantially homologous" when at least about 60% (preferably at least about 80%, and most preferably at least about 90 or 95%) of the nucleotides match over the defined length of the DNA sequences. Sequences that are substantially homologous can be identified by comparing the sequences using standard software available in sequence data banks, or in a Southern hybridization experiment under, for example, stringent conditions as defined for that particular system. Defining appropriate hybridization conditions is within the skill of the art. See, e.g., Maniatis et al., supra; DNA Cloning, Vols. I & II, supra; Nucleic Acid Hybridization, supra.

As used herein an amino acid sequence is 100% "homologous" to a second amino acid sequence if the two amino acid sequences are identical, and/or differ only by neutral or conservative substitutions as defined below. Accordingly, an amino acid sequence is 50% "homologous" to a second amino acid sequence if 50% of the two amino acid sequences are identical, and/or differ only by neutral or conservative substitutions.

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As used herein, DNA and protein sequence percent identity can be determined using MacVector 6.0.1, Oxford Molecular Group PLC (1996) and the Clustal W algorithm with the alignment default parameters, and default parameters for identity. These

commercially available programs can also be used to determine sequence similarity using the same or analogous default parameters.

The term "corresponding to" is used herein to refer similar or homologous sequences, whether the exact position is identical or different from the molecule to which the similarity or homology is measured. Thus, the term "corresponding to" refers to the sequence similarity, and not the numbering of the amino acid residues or nucleotide bases.

As used herein a "heterologous nucleotide sequence" is a nucleotide sequence that is added to a nucleotide sequence of the present invention by recombinant methods to form a nucleic acid which is not naturally formed in nature. Such nucleic acids can encode fusion proteins or peptides, including chimeric proteins and peptides. Thus the heterologous nucleotide sequence can encode peptides and/or proteins which contain regulatory and/or structural properties. In another such embodiment the heterologous nucleotide can encode a protein or peptide that functions as a means of detecting the protein or peptide encoded by the nucleotide sequence of the present invention after the recombinant nucleic acid is expressed. In still another such embodiment the heterologous nucleotide can function as a means of detecting a nucleotide sequence of the present invention. A heterologous nucleotide sequence can comprise non-coding sequences including restriction sites, regulatory sites, promoters and the like.

The present invention also relates to cloning vectors containing nucleic acids encoding analogs and derivatives of the bromodomains of the present invention and polypeptides/peptides that can bind a bromodomain when a lysine of the polypeptide/peptide is acetylated, including modified fragments, that have the same or homologous functional activity as the individual fragments, and homologs thereof. The production and use of derivatives and analogs related to the fragments are within the scope of the present invention.

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Due to the degeneracy of nucleotide coding sequences, other DNA sequences which encode substantially the same amino acid sequence as a nucleic acid encoding a protein

comprising bromodomain or bromodomain binding partner (i.e., when posttranscriptionally acetylated) of the present invention for example, may be used in the practice of the present invention. These include but are not limited to allelic genes, homologous genes from other species, which are altered by the substitution of different codons that encode the same amino acid residue within the sequence, thus producing a silent change. Likewise, the peptides and polypeptides of the present invention include, but are not limited to, those containing, as a primary amino acid sequence, analogous portions of their respective amino acid sequences including altered sequences in which functionally equivalent amino acid residues are substituted for 10 residues within the sequence resulting in a conservative amino acid substitution. For example, one or more amino acid residues within the sequence can be substituted by another amino acid of a similar polarity, which acts as a functional equivalent, resulting in a silent alteration. Substitutes for an amino acid within the sequence may be selected from other members of the class to which the amino acid belongs. For example, the nonpolar (hydrophobic) amino acids include alanine, leucine, isoleucine, 15 valine, proline, phenylalanine, tryptophan and methionine. Amino acids containing aromatic ring structures are phenylalanine, tryptophan, and tyrosine. The polar neutral amino acids include glycine, serine, threonine, cysteine, tyrosine, asparagine, and glutamine. The positively charged (basic) amino acids include arginine, and lysine. 20 The negatively charged (acidic) amino acids include aspartic acid and glutamic acid.

Particularly preferred conserved amino acid exchanges are:

- (a) Lys for Arg or vice versa such that a positive charge may be maintained;
- (b) Glu for Asp or vice versa such that a negative charge may be maintained;
- 25 (c) Ser for Thr or vice versa such that a free -OH can be maintained;
 - (d) Gln for Asn or vice versa such that a free NH₂ can be maintained;
 - (e) Ile for Leu or for Val or vice versa as roughly equivalent hydrophobic amino acids; and
 - (f) Phe for Tyr or vice versa as roughly equivalent aromatic amino acids.

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A conservative change generally leads to less change in the structure and function of the resulting protein. A non-conservative change is more likely to alter the structure, activity or function of the resulting protein. The present invention should be considered to include sequences containing conservative changes which do not significantly alter the activity or binding characteristics of the resulting protein. Specific amino acid residues for the P/CAF bromodomain have been identified that are important for binding, indicating a potential lower stringency for the substitution of the remaining amino acids residues.

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All of the peptides/fragments of the present invention can be modified by being placed in a fusion or chimeric peptide or protein, or labeled e.g., to have an N-terminal FLAG10 tag, or H6 tag. In a particular embodiment the P/CAF bromodomain fragment can be modified to contain a marker protein such as green fluorescent protein as described in U.S. Patent No. 5,625,048 filed April 29, 1997 and WO 97/26333, published July 24, 1997 each of which are hereby incorporated by reference herein in their entireties.

- The nucleic acids encoding peptides and protein fragments of the present invention and 15 analogs thereof can be produced by various methods known in the art. The manipulations which result in their production can occur at the gene or protein level [Sambrook et al., 1989, supra]. The nucleotide sequence can be cleaved at appropriate sites with restriction endonuclease(s), followed by further enzymatic modification if 20 desired, isolated, and ligated in vitro. In addition a nucleic acid sequence can be mutated in vitro or in vivo, to create and/or destroy translation, initiation, and/or termination sequences, or to create variations in coding regions and/or form new restriction endonuclease sites or destroy preexisting ones, to facilitate further in vitro modification. Any technique for mutagenesis known in the art can be used, including 25 but not limited to, in vitro site-directed mutagenesis [Hutchinson et al., J. Biol. Chem., 253:6551 (1978); Zoller and Smith, DNA, 3:479-488 (1984); Oliphant et al., Gene, 44:177 (1986); Hutchinson et al., Proc. Natl. Acad. Sci. U.S.A., 83:710 (1986)], use of TAB® linkers (Pharmacia), etc. PCR techniques are preferred for site directed mutagenesis [see Higuchi, 1989, "Using PCR to Engineer DNA", in PCR Technology: Principles and Applications for DNA Amplification, H. Erlich, ed., Stockton Press,
- 30 Principles and Applications for DNA Amplification, H. Erlich, ed., Stockton Press, Chapter 6, pp. 61-70].

The identified and isolated nucleic acids can then be inserted into an appropriate cloning vector. A large number of vector-host systems known in the art may be used.

Protein expression and purification

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A bacterial protein expression system can be used to make various stable isotopically labeled (¹³C, ¹⁵N, and ²H) protein samples that are useful for a three-dimensional NMR structural determination of a protein complex. For example a pET14b (Novagen) bacterial expression vector can be constructed which expresses the recombinant P/CAF bromodomain as an amino-terminal His-tagged fusion protein.

Protein expression and purification can be conducted using standard procedures for His-tagged proteins [Zhou et al., J. Biol. Chem. 270:31119-31123 (1995)]. To optimize the level of protein expression, various bacterial growth and expression conditions can be screened, which include different E. Coli cell lines, and growth and protein induction temperatures. Generally, it is preferred to obtain the maximum amount of soluble protein while still inducing protein expression with a relatively low IPTG concentration e.g., ~0.2mM (final concentration) at 16°C. As exemplified below, the bromodomain of P/CAF (residues 719-832 of SEQ ID NO:2 which is SEQ ID NO:7) was subcloned into the pET14b expression vector (Novagen) and expressed in Escherichia coli BL21(DE3) cells. Uniformly ¹⁵N- and ¹⁵N/¹³C-labeled proteins were prepared by growing bacteria in a minimal medium containing ¹⁵NH₄Cl with or without ¹³C₆-glucose. A uniformly ¹⁵N/¹³C-labeled and fractionally deuterated protein sample was prepared by growing the cells in 75% ²H₂O. The bromodomain was purified by affinity chromatography on a nickel-IDA column (Invitrogen) followed by the removal of poly-His tag by thrombin cleavage. The final purification of the protein was achieved by size-exclusion chromatography. The acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation. NMR samples contained approximately 1 mM protein in 100mM phosphate buffer of pH 6.5 and 5mM perdeuterated DTT and 0.5mM EDTA in $H_2O/^2H_2O$ (9/1) or 2H_2O .

One major advantage of using the heteronuclear multidimensional approach, as exemplied herein, is that the NMR resonance assignments of a protein are obtained in a sequence-specific manner which assures accuracy and greatly facilitates data analysis and structure determination [Clore, G. M. & Gronenborn, A. M. Meth. Enzymol.

- 5 239:249-363 (1994)]. In addition, the signal overlapping problems in the protein spectra are minimized by the use of multidimensional NMR spectra, which separates the proton signals according to the chemical shifts of their attached hetero-nuclei (such as ¹⁵N and ¹³C). This NMR approach has been proven very powerful for structural analysis of large proteins [Clore, G. M. & Gronenborn, A. M. Meth. Enzymol.
- 239:249-363 (1994)]. To facilitate sequence-specific resonance assignments for the structural study, a uniformly ¹³C, ¹⁵N-labeled and fractionally (75%) deuterated protein sample of the bromodomain can be prepared by growing bacterial cells in 75% ²H₂O as exemplified below. Such protein samples can be used for triple-resonance NMR experiments. A triple-labeled protein sample is useful for high-resolution NMR structural studies. Because of the favorable ¹H, ¹³C, and ¹⁵N relaxation rates caused by

the partial deuteration of the protein, constant-time triple-resonance NMR spectra can be acquired with higher digital resolution and sensitivity [Sattler, M. & Fesik, S. W. *Structure* 4:1245-1249 (1996)]. In addition, various stable-isotopically labeled (¹⁵N and ¹³C /¹⁵N) proteins can also be prepared using this procedure.

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Synthetic Polypeptides

The term "polypeptide" is used in its broadest sense to refer to a compound of two or more subunit amino acids, amino acid analogs, or peptidomimetics. The subunits are linked by peptide bonds. The terms "polypeptide", "protein", and "peptide" are used interchangeably herein, though preferably as used herein a "peptide" refers to a compound of at least two but less than fifty subunit amino acids, and a polypeptide or protein refers to compound of fifty or more amino acids. The polypeptides of the present invention may be chemically synthesized or as detailed above, genetically engineered or isolated from natural sources.

In addition, potential drugs or agents that may be tested in the drug screening assays of the present invention may also be chemically synthesized. When the peptide is to be modified, e.g., acetylated, the modification can be at any time during the peptide synthesis, including using an acetyl-lysine as a starting material or acetylating a lysine residue of a peptide after the peptide has been synthesized. In the Example below, the acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation.

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Thus, synthetic polypeptides, prepared using the well known techniques of solid phase, liquid phase, or peptide condensation techniques, or any combination thereof, can include natural and unnatural amino acids. Amino acids used for peptide synthesis may be standard Boc (N^{α} -amino protected N^{α} -t-butyloxycarbonyl) amino acid resin with the standard deprotecting, neutralization, coupling and wash protocols of the original solid phase procedure of Merrifield [J. Am. Chem. Soc., 85:2149-2154 (1963)], or the base-labile N^{α} -amino protected 9-fluorenylmethoxycarbonyl (Fmoc) amino acids first described by Carpino and Han [J. Org. Chem., 37:3403-3409 (1972)]. Both Fmoc and Boc N^α-amino protected amino acids can be obtained from Fluka, Bachem, Advanced Chemtech, Sigma, Cambridge Research Biochemical, Bachem, or Peninsula Labs or other chemical companies familiar to those who practice this art. In addition, the method of the invention can be used with other N°-protecting groups that 20 are familiar to those skilled in this art. Solid phase peptide synthesis may be accomplished by techniques familiar to those in the art and provided, for example, in Stewart and Young [Solid Phase Synthesis, Second Edition, Pierce Chemical Co., Rockford, IL (1984)] and Fields and Noble [Int. J. Pept. Protein Res., 35:161-214 (1990)], or using automated synthesizers, such as sold by ABS. Thus, polypeptides of the invention may comprise D-amino acids, a combination of D- and L-amino acids, 25 and various "designer" amino acids (e.g., β-methyl amino acids, Cα-methyl amino acids, and Nα-methyl amino acids, etc.) to convey special properties. Synthetic amino acids include ornithine for lysine, fluorophenylalanine for phenylalanine, and norleucine for leucine or isoleucine. Additionally, by assigning specific amino acids at specific coupling steps, α -helices, β turns, β sheets, γ -turns, and cyclic peptides can be 30 generated.

In a further embodiment, subunits of peptides that confer useful chemical and structural properties will be chosen. For example, peptides comprising D-amino acids will be resistant to L-amino acid-specific proteases in vivo. In addition, the present invention envisions preparing peptides that have more well defined structural properties, and the use of peptidomimetics, and peptidomimetic bonds, such as ester bonds, to prepare peptides with novel properties. In another embodiment, a peptide may be generated that incorporates a reduced peptide bond, i.e., R₁-CH₂-NH-R₂, where R₁ and R₂ are amino acid residues or sequences. A reduced peptide bond may be introduced as a dipeptide subunit. Such a molecule would be resistant to peptide bond hydrolysis, e.g., protease activity. Such peptides would provide ligands with unique function and activity, such as extended half-lives in vivo due to resistance to metabolic breakdown, or protease activity. Furthermore, it is well known that in certain systems constrained peptides show enhanced functional activity [Hruby, Life Sciences, 31:189-199 (1982); Hruby et al., Biochem J., 268:249-262 (1990)]; the present invention provides a method to produce a constrained peptide that incorporates random sequences at all other positions.

Constrained and cyclic peptides. A constrained, cyclic or rigidized peptide may be prepared synthetically, provided that in at least two positions in the sequence of the peptide an amino acid or amino acid analog is inserted that provides a chemical functional group capable of crosslinking to constrain, cyclise or rigidize the peptide after treatment to form the crosslink. Cyclization will be favored when a turn-inducing amino acid is incorporated. Examples of amino acids capable of crosslinking a peptide are cysteine to form disulfides, aspartic acid to form a lactone or a lactam, and a chelator such as γ-carboxyl-glutamic acid (Gla) (Bachem) to chelate a transition metal and form a cross-link. Protected γ-carboxyl glutamic acid may be prepared by modifying the synthesis described by Zee-Cheng and Olson [Biophys. Biochem. Res. Commun., 94:1128-1132 (1980)]. A peptide in which the peptide sequence comprises at least two amino acids capable of crosslinking may be treated, e.g., by oxidation of cysteine residues to form a disulfide or addition of a metal ion to form a chelate, so as to crosslink the peptide and form a constrained, cyclic or rigidized peptide.

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The present invention provides strategies to systematically prepare cross-links. For example, if four cysteine residues are incorporated in the peptide sequence, different protecting groups may be used (Hiskey, in The Peptides: Analysis, Synthesis, Biology, Vol. 3, Gross and Meienhofer, eds., Academic Press: New York, pp. 137-167 (1981);

Ponsanti et al., Tetrahedron, 46:8255-8266 (1990)]. The first pair of cysteines may be deprotected and oxidized, then the second set may be deprotected and oxidized. In this way a defined set of disulfide cross-links may be formed. Alternatively, a pair of cysteines and a pair of chelating amino acid analogs may be incorporated so that the cross-links are of a different chemical nature.

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Non-classical amino acids that induce conformational constraints. The following non-classical amino acids may be incorporated in the peptide in order to introduce particular conformational motifs: 1,2,3,4-tetrahydroisoquinoline-3-carboxylate [Kazmierski et al., J. Am. Chem. Soc., 113:2275-2283 (1991)]; (2S,3S)-methyl-phenylalanine (2S,3R)-methyl-phenylalanine (2

phenylalanine, (2S,3R)-methyl-phenylalanine, (2R,3S)-methyl-phenylalanine and (2R,3R)-methyl-phenylalanine (Kazmierski and Hruby, *Tetrahedron Lett.* (1991)]; 2-aminotetrahydronaphthalene-2-carboxylic acid [Landis, Ph.D. Thesis, University of Arizona (1989)]; hydroxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylate [Miyake *et al.*, *J. Takeda Res. Labs.*, **43:**53-76 (1989)]; β-carboline (D and L) [Kazmierski, Ph.D.

Thesis, University of Arizona (1988)]; HIC (histidine isoquinoline carboxylic acid) [Zechel et al., Int. J. Pep. Protein Res., 43 (1991)]; and HIC (histidine cyclic urea) (Dharanipragada).

The following amino acid analogs and peptidomimetics may be incorporated into a

25 peptide to induce or favor specific secondary structures: LL-Acp (LL-3-amino2-propenidone-6-carboxylic acid), a β-turn inducing dipeptide analog [Kemp et al., J.

Org. Chem., 50:5834-5838 (1985)]; β-sheet inducing analogs [Kemp et al.,

Tetrahedron Lett., 29:5081-5082 (1988); β-turn inducing analogs [Kemp et al.,

Tetrahedron Lett., 29:5057-5060 (1988)]; α-helix inducing analogs (Kemp et al.,

Tetrahedron Lett., 29:4935-4938 (1988)]; γ-turn inducing analogs [Kemp et al., J.

Org. Chem., 54:109:115 (1989)]; and analogs provided by the following references:

Nagai and Sato, Tetrahedron Lett., 26:647-650 (1985); DiMaio et al., J. Chem. Soc.

Perkin Trans., p. 1687 (1989); also a Gly-Ala turn analog [Kahn et al., Tetrahedron

spectra of mutated proteins can be compared to that of the wild-type protein bromodomain.

Chemical-shift perturbations due to ligand binding have proven to be a reliable and sensitive probe for the ligand binding site of the protein. This is because the chemicalshift changes of the backbone amide groups are likely to reflect any changes in protein conformation and/or hydrogen bonding due to the peptide/ligand binding. To examine the effects of a mutation on the ligand binding (in this case the ligand is a peptide comprising an acetyl-lysine), peptide titration experiments can be conducted by following the changes of ¹H/¹⁵N signals of the mutant proteins as a function of the 10 peptide concentration. These experiments indicate whether the acetyl-lysine binding site remains the same or changes in the mutants relative to the wild type protein. The effects of the mutation on the peptide binding affinity can also be examined by NMR spectroscopy. If the mutated proteins result in the reduction of the binding affinity, a change of the exchange phenomenon between the free and the ligand-bound signals should be observed in NMR spectrum. If the reduction in binding affinity causes the peptide binding to change from a slow exchange rate to a fast exchange rate, on the NMR time scale, then the peptide binding affinity can be determined from the NMR titration experiment. From these mutation analyses key amino acid residues that are important for binding a peptide comprising the acetyl-lysine can be identified. Such 20 analysis has been exemplified below.

Protein Structure Determination by NMR Spectroscopy

The NMR results from the present invention are summarized by the atomic structure coordinates of the free form of the P/CAF bromodomain (Table 5) and of the P/CAF bromodomain-acetyl-histamine complex (Table 6). The NMR chemical shift assignments of the P/CAF bromodomain are included in the chemical shift table (Table 1) for the ¹H-¹⁵N HSQC spectrum of P/CAF bromodomain. The unambiguous NOE-derived Inter-proton Distance Restraints are in Table 2, the ambiguous NOE-derived Inter-proton Distance Restraints are in Table 3, and the ¹H bonding restraints are disclosed in Table 4.

Backbone and Side-chain Assignments: Sequence-specific backbone assignment can be achieved by using a suite of deuterium-decoupled triple-resonance 3D NMR experiments which include HNCA, HN(CO)CA, HN(CA)CB, HN(COCA)CB, HNCO, and HN(CA)CO experiments [Yamazaki, et al., J. Am. Chem. Soc. 116:11655-11666 (1994)]. The water flip-back scheme is used in these NMR pulse programs to minimize amide signal attenuation from water exchange. Sequential side-chain assignments are typically accomplished from a series of 3D NMR experiments with alternative approaches to confirm the assignments. These experiments include 3D ¹⁵N TOCSY-HSQC, HCCH-TOCSY, (H)C(CO)NH-TOCSY, and H(C)(CO)NH-TOCSY [see Clore, G. M. & Gronenborn, A. M. Meth. Enzymol. 239:249-363 (1994);Sattler et al., Prog. in Nuclear Magnetic Resonance Spec. 4:93-158 (1999)].

Stereospecific Methyl Groups: Stereospecific assignments of methyl groups of Valine and Leucine residues can be obtained from an analysis of carbon signal multiplet splitting using a fractionally ¹³C-labeled protein sample, which can be readily prepared using M9 minimal medium containing 10% ¹³C-/90% ¹²C-glucose mixture [see Neri, et al., Biochemistry 28:7510-7516 (1989)].

Dihedral Angle Restraints: Backbone dihedral angle (Φ) constraints can be generated from the ${}^3J_{\text{HNH}\alpha}$ coupling constants measured in a HNHA-J experiment [see Vuister, G. & Bax, A. J. Am. Chem. Soc. 115:7772-7777 (1993)]. Side-chain dihedral angles (χ1) can be obtained from short mixing time ${}^{15}\text{N}$ -edited 3D TOCSY-HSQC [see Clore, et al., J. Biomol. NMR 1:13-22 (1991)] and 3D HNHB experiments [see Matson et al., J. Biomol. NMR 3:239-244 (1993)], which can also provide stereospecific assignments of β methylene protons.

Hydrogen Bonds Restraints: Amide protons that are involved in hydrogen bonds can be identified from an analysis of amide exchange rates measured from a series of 2D ¹H/¹⁵N HSQC spectra recorded after adding ²H₂O to the protein sample.

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NOE Distance Restraints: Distance restraints are obtained from analysis of ¹⁵N, and ¹³C-edited 3D NOESY data, which can be collected with different mixing times to minimize spin diffusion problems. The nuclear Overhauser effect (NOE)-derived

restraints are categorized as strong (1.8-3 Å), medium (1.8-4 Å) or weak (1.8-5 Å) based on the observed NOE intensities. A recently developed procedure for the iterative automated NOE analysis by using ARIA [see Nilges et al., Prog. NMR Spectroscopy 32:107-139 (1998)] can be employed which integrates with X-PLOR for structural calculations. To ensure the success of ARIA/X-PLOR-assisted NOE analysis and structure calculations, the ARIA assigned NOE peaks can be manually confirmed.

Intermolecular NOE Distance Restrains: For the structural determination of a protein/peptide complex, intermolecular NOE distance restraints can be obtained from a 13 C-edited (F_1) and 15 N, and 13 C-filtered (F_3) 3D NOESY data set collected for a sample containing isotope-labeled protein and non-labeled peptide.

Structure Calculations and Refinements: Structures of the protein can be generated using a distance geometry/simulated annealing protocol with the X-PLOR program

[see Nilges, et al., FEBS Lett. 229:317-324 (1988); Kuszewski, et al., J. Biolmol. NMR
2:33-56 (1992); Brünger, A. T. X-PLOR Version 3.1: A system for X-Ray crystallography and NMR (Yale University Press, New Haven, CT, 1993)]. The structure calculations can employ inter-proton distance restraints obtained from 15N-and 13C-resolved NOESY spectra. The initial low-resolution structures can be used to facilitate NOE assignments, and help identify hydrogen bonding partners for slowly exchanging amide protons. The experimental restraints of dihedral angles and hydrogen bonds can be included in the distance restraints for structure refinements.

<u>Protein-Structure Based Design of Agonists and Antagonists</u> <u>of the Bromodomain-Acetyl-Lysine Binding Complex</u>

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Once the three-dimensional structure of the Bromodomain and the Bromodomain-acetyl-lysine binding complex are determined, a potential drug or agent (antagonist or agonist) can be examined through the use of computer modeling using a docking program such as GRAM, DOCK, or AUTODOCK [Dunbrack et al., 1997, supra]. This procedure can include computer fitting of potential agents to the bromodomain, for example, to ascertain how well the shape and the chemical structure of the potential ligand will complement or interfere with the interaction between the bromodomain and

the acetyl-lysine [Bugg et al., Scientific American, Dec.:92-98 (1993); West et al., TIPS, 16:67-74 (1995)]. Computer programs can also be employed to estimate the attraction, repulsion, and steric hindrance of the agent to the dimer-dimer binding site, for example. Generally the tighter the fit (e.g., the lower the steric hindrance, and/or the greater the attractive force) the more potent the potential drug will be since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interfere with related proteins. This will minimize potential side-effects due to unwanted interactions with other proteins.

Initially a potential drug could be obtained by screening a random peptide library produced by recombinant bacteriophage for example, [Scott and Smith, Science, 249:386-390 (1990); Cwirla et al., Proc. Natl. Acad. Sci., 87:6378-6382 (1990); Devlin et al., Science, 249:404-406 (1990)] or a chemical library. An agent selected in this manner could be then be systematically modified by computer modeling programs until one or more promising potential drugs are identified. Such analysis has been shown to be effective in the development of HIV protease inhibitors [Lam et al., Science 263:380-384 (1994); Wlodawer et al., Ann. Rev. Biochem. 62:543-585 (1993); Appelt, Perspectives in Drug Discovery and Design 1:23-48 (1993); Erickson, Perspectives in Drug Discovery and Design 1:109-128 (1993)].

Such computer modeling allows the selection of a finite number of rational chemical modifications, as opposed to the countless number of essentially random chemical modifications that could be made, any one of which might lead to a useful drug. Each chemical modification requires additional chemical steps, which while being reasonable for the synthesis of a finite number of compounds, quickly becomes overwhelming if all possible modifications needed to be synthesized. Thus, through the use of the three-dimensional structural analysis disclosed herein and computer modeling, a large number of these compounds can be rapidly screened on the computer monitor screen, and a few likely candidates can be determined without the laborious synthesis of untold numbers of compounds.

Once a potential drug (agonist or antagonist) is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential drug may be synthesized *de novo*. As mentioned above, the *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

The potential drug can then be tested in any standard binding assay (including in high throughput binding assays) for its ability to bind to the ZA loop of a bromodomain.

Alternatively the potential drug can be tested for its ability to modulate the binding of a bromodomain to acetylated histamine, for example. When a suitable potential drug is identified, a second NMR structural analysis can optionally be performed on the binding complex formed between the bromodomain-acetyl-lysine binding complex, or the bromodomain alone and the potential drug. Computer programs that can be used to aid in solving such three-dimensional structures include QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODE, and ICM, MOLMOL, RASMOL, AND GRASP [Kraulis, J. Appl Crystallogr. 24:946-950 (1991)]. Most if not all of these programs and others as well can be also obtained from the WorldWideWeb through the internet.

Using the approach described herein and equipped with the structural analysis disclosed herein, the three-dimensional structures of other bromodomain-acetyl-lysine binding complexes can more readily be obtained and analyzed. Such analysis will, in turn, allow corresponding drug screening methodology to be performed using the three-dimensional structures of such related complexes.

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For all of the drug screening assays described herein further refinements to the structure of the drug will generally be necessary and can be made by the successive iterations of any and/or all of the steps provided by the particular drug screening assay, including further structural analysis by NMR, for example.

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Phage libraries for Drug Screening.

Phage libraries have been constructed which when infected into host *E. coli* produce random peptide sequences of approximately 10 to 15 amino acids [Parmley and Smith,

Gene 73:305-318 (1988), Scott and Smith, Science 249:386-249 (1990)]. Specifically, the phage library can be mixed in low dilutions with permissive E. coli in low melting point LB agar which is then poured on top of LB agar plates. After incubating the plates at 37°C for a period of time, small clear plaques in a lawn of E. coli will form which represents active phage growth and lysis of the E. coli. A representative of these phages can be absorbed to nylon filters by placing dry filters onto the agar plates. The filters can be marked for orientation, removed, and placed in washing solutions to block any remaining absorbent sites. The filters can then be placed in a solution containing, for example, a radioactive bromodomain. After a specified incubation period, the filters can be thoroughly washed and developed for autoradiography. Plaques containing the phage that bind to the radioactive bromodomain can then be identified. These phages can be further cloned and then retested for their ability to bind to the bromodomain as before. Once the phage has been purified, the binding sequence contained within the phage can be determined by standard DNA sequencing techniques. Once the DNA sequence is known, synthetic peptides can be generated which are encoded by these sequences. These peptides can be tested, for example, for their ability to modulate the affinity of the bromodomain for its binding partner (e.g., a protein comprising an acetyl-lysine or a fragment of that protein).

The effective peptide(s) can be synthesized in large quantities for use in *in vivo* models and eventually in humans to treat certain tumors. It should be emphasized that synthetic peptide production is relatively non-labor intensive, easily manufactured, quality controlled and thus, large quantities of the desired product can be produced quite cheaply. Similar combinations of mass produced synthetic peptides have been used with great success [Patarroyo, *Vaccine*, 10:175-178 (1990)].

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Drug Screening Assays

The drug screening assays of the present invention may use any of a number of means for determining the interaction between an agent or drug and a peptide comprising an acetyl-lysine and/or a bromodomain. Thus, standard high throughput drug screening procedures can be employed using a library of low molecular weight compounds, for

example that can be screened to identify a binding partner for the bromodoamin. Any such chemical library can be used including those discussed above.

In a particular assay, a bromodomain is placed on or coated onto a solid support.

Methods for placing the peptides or proteins on the solid support are well known in the art and include such things as linking biotin to the protein and linking avidin to the solid support. An agent is allowed to equilibrate with the bromodomain to test for binding. Generally, the solid support is washed and agents that are retained are selected as potential drugs. Alternatively, a peptide comprising an acetyl-lysine is placed on or coated onto a solid support. In a particular embodiment of this type, the peptide comprises the amino acid sequence of SEQ ID NO:4.

The agent may be labeled. For example, in one embodiment radiolabeled agents are used to measure the binding of the agent. In another embodiment the agents have fluorescent markers. In yet another embodiment, a Biocore chip (Pharmacia) coated with the bromodomain is used, for example and the change in surface conductivity can be measured.

In addition, since a number of proteins have been identified that contain

20 bromodomains, and the binding partners of many of these proteins are known, the fact that the bromodomain specifically binds to an acetylated lysine as disclosed herein allows the identification and preparation of a number of potential modulators of the bromodomain-acetyl-lysine binding complex based on the amino acid sequences of the binding partners to the proteins. Such potential modulators include: ISYGR-AcK-

25 KRRQRR (SEQ ID NO:4), ARKSTGG-AcK-APRKQL (SEQ ID NO:5) and QSTSRHK-AcK-LMFKTE (SEQ ID NO:6) which bind to the P/CAF bromodomain as shown in the Example, below. Such peptides also can be used, for example, as a starting point for the design of an inhibitor of the bromodomain-acetyl-lysine binding complex.

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Alternatively, a drug can be specifically designed to bind to the ZA loop of a bromodomain for example, such as the P/CAF bromodomain, and be assayed through NMR based methodology [Shuker et al., Science 274:1531-1534 (1996) hereby

incorporated by reference in its entirety.] In a particular embodiment, analogs of the binding partner of the bromodomain can be used in this analysis. One such peptide has the amino acid sequence of SEQ ID NO:4. In another embodiment of this type, the peptide has the amino acid sequence of SEQ ID NO:5. In another such embodiment of this type, the peptide has the amino acid sequence of SEQ ID NO:6.

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The assay begins with contacting a compound with a ¹⁵N-labeled bromodomain. Binding of the compound with the ZA loop of the bromodomain can be determined by monitoring the ¹⁵N- or ¹H-amide chemical shift changes in two dimensional ¹⁵Nheteronuclear single-quantum correlation (15N-HSQC) spectra upon the addition of the compound to the ¹⁵N-labeled bromodomain. Since these spectra can be rapidly obtained, it is feasible to screen a large number of compounds [Shuker et al., Science 274:1531-1534 (1996)]. A compound is identified as a potential ligand if it binds to the ZA loop of the bromodomain. In a further embodiment, the potential ligand can then be used as a model structure, and analogs to the compound can be obtained (e.g., from the vast chemical libraries commercially available, or alternatively through de novo synthesis). The analogs are then screened for their ability to bind the ZA loop of the bromodomain thus to obtain a ligand. An analog of the potential ligand is chosen as a ligand when it binds to the ZA loop of the bromodomain with a higher binding affinity than the potential ligand. In a preferred embodiment of this type the analogs are screened by monitoring the 15N- or 1H-amide chemical shift changes in two dimensional ¹⁵N-heteronuclear single-quantum correlation (¹⁵N-HSQC) spectra upon the addition of the analog to the ¹⁵N-labeled bromodomain as described above.

In another further embodiment, compounds are screened for binding to two nearby sites on the bromodomain. In this case, a compound that binds a first site of the bromodomain does not bind a second nearby site. Binding to the second site can be determined by monitoring changes in a different set of amide chemical shifts in either the original screen or a second screen conducted in the presence of a ligand (or potential ligand) for the first site. From an analysis of the chemical shift changes the approximate location of a potential ligand for the second site is identified. Optimization of the second ligand for binding to the site is then carried out by screening structurally related compounds (e.g., analogs as described above). When

ligands for the first site and the second site are identified, their location and orientation in the ternary complex can be determined experimentally either by NMR spectroscopy or X-ray crystallography. On the basis of this structural information, a linked compound is synthesized in which the ligand for the first site and the ligand for the second site are linked. In a preferred embodiment of this type the two ligands are covalently linked. This linked compound is tested to determine if it has a higher binding affinity for the bromodomain than either of the two individual ligands. A linked compound is selected as a ligand when it has a higher binding affinity for the bromodomain than either of the two ligands. In a preferred embodiment the affinity of the linked compound with the bromodomain is determined monitoring the ¹⁵N- or ¹H-amide chemical shift changes in two dimensional ¹⁵N-heteronuclear single-quantum correlation (¹⁵N-HSQC) spectra upon the addition of the linked compound to the ¹⁵N-labeled bromodomain as described above.

15 A larger linked compound can be constructed in an analogous manner, e.g., linking three ligands which bind to three nearby sites on the bromodomain to form a multilinked compound that has an even higher affinity for the bromodomain than the linked compound.

20 <u>Identification of New Bromodomains</u>

By disclosing that protein bound acetyl-lysine is a binding partner for bromodomains, the present invention provides a method of identifying novel proteins that contain bromodomains. In short, a protein fragment or analog thereof comprising an acetyllysine can be used as bait to identify a binding partner that comprises a bromodomain. Any one of a number of procedures can be carried out to identify such a binding partner. One such assay comprises passing a cell extract over the bait peptide which is attached to a solid support. After washing the solid support to remove any non-specific binders, the bromodomain containing protein can be eluted from the solid support with an appropriate eluant. In a particular embodiment, the free bait peptide can be used in the elution. Other methodology includes the use of a yeast two-hybrid system, a GST pull down assay, ELISA, immunometric assays, and a modification of the CORT procedure of Schlessinger *et al.*, (US Patent No. 5,858,686, Issued on

January 12, 1999 which is hereby incorporated by reference in its entirety) for use with the bromodomain-acetyl-lysine binding complex.

Labels:

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Suitable labels include enzymes, fluorophores (e.g., fluorescein isothiocyanate (FITC), phycoerythrin (PE), Texas red (TR), rhodamine, free or chelated lanthanide series salts, especially Eu³⁺, to name a few fluorophores), chromophores, radioisotopes, chelating agents, dyes, colloidal gold, latex particles, ligands (e.g., biotin), and chemiluminescent agents. When a control marker is employed, the same or different labels may be used for the test and control marker gene.

In the instance where a radioactive label, such as the isotopes ³H, ¹⁴C, ³²P, ³⁵S, ³⁶Cl, ⁵¹Cr, ⁵⁷Co, ⁵⁸Co, ⁵⁹Fe, ⁹⁰Y, ¹²⁵I, ¹³¹I, and ¹⁸⁶Re are used, known currently available counting procedures may be utilized. In the instance where the label is an enzyme, detection may be accomplished by any of the presently utilized colorimetric, spectrophotometric, fluorospectrophotometric, amperometric or gasometric techniques known in the art.

20 Direct labels are one example of labels which can be used according to the present invention. A direct label has been defined as an entity, which in its natural state, is readily visible, either to the naked eye, or with the aid of an optical filter and/or applied stimulation, e.g. U.V. light to promote fluorescence. Among examples of colored labels, which can be used according to the present invention, include metallic sol 25 particles, for example, gold sol particles such as those described by Leuvering (U.S. Patent 4,313,734); dye sole particles such as described by Gribnau et al. (U.S. Patent 4,373,932 and May et al. (WO 88/08534); dyed latex such as described by May, supra, Snyder (EP-A 0 280 559 and 0 281 327); or dyes encapsulated in liposomes as described by Campbell et al. (U.S. Patent 4,703,017). Other direct labels include a radionucleotide, a fluorescent moiety or a luminescent moiety. In addition to these 30 direct labeling devices, indirect labels comprising enzymes can also be used according to the present invention. Various types of enzyme linked immunoassays are well known in the art, for example, alkaline phosphatase and horseradish peroxidase,

lysozyme, glucose-6-phosphate dehydrogenase, lactate dehydrogenase, urease, these and others have been discussed in detail by Eva Engvall in Enzyme Immunoassay ELISA and EMIT in *Methods in Enzymology*, **70**:419-439 (1980) and in U.S. Patent 4,857,453.

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Suitable enzymes include, but are not limited to, alkaline phosphatase, β -galactosidase, green fluorescent protein and its derivatives, luciferase, and horseradish peroxidase.

Other labels for use in the invention include magnetic beads or magnetic resonance imaging labels.

Antibodies to Portions of the Bromodomain that Interact with Acetyl-Lysine

According to the present invention, the bromodomains, and more particularly the ZA loops of the bromodomains and fragments thereof can be produced by a recombinant source, or through chemical synthesis, or through the modification of these peptides and fragments; and derivatives or analogs thereof, including fusion proteins, may be used as an immunogen to generate antibodies that specifically interfere with the formation of the bromodomain-acetyl-lysine binding complex. Similarly, antibodies can be raised against peptides that comprise one or more acetyl-lysine residues which also interfere with the formation of the bromodomain-acetyl-lysine binding complex. Such antibodies include but are not limited to polyclonal, monoclonal, chimeric, single chain, Fab fragments, and a Fab expression library.

Various procedures known in the art may be used for the production of the polyclonal antibodies. For the production of antibody, various host animals can be immunized by injection with the peptide having the amino acid sequence of SEQ ID NO:3, for example, or a derivative (e.g., or fusion protein) thereof, including but not limited to rabbits, mice, rats, sheep, goats, etc. In one embodiment, the peptide can be conjugated to an immunogenic carrier, e.g., bovine serum albumin (BSA) or keyhole limpet hemocyanin (KLH). Various adjuvants may be used to increase the immunological response, depending on the host species, including but not limited to Freund's (complete and incomplete), mineral gels such as aluminum hydroxide, surface

active substances such as lysolecithin, pluronic polyols, polyanions, peptides, oil emulsions, keyhole limpet hemocyanins, dinitrophenol, and potentially useful human adjuvants such as BCG (bacille Calmette-Guerin) and Corynebacterium parvum.

For preparation of monoclonal antibodies directed toward the peptides or protein 5 fragments of the present invention, or analog, or derivative thereof, any technique that provides for the production of antibody molecules by continuous cell lines in culture may be used. These include but are not limited to the hybridoma technique originally developed by Kohler and Milstein [Nature, 256:495-497 (1975)], as well as the trioma 10 technique, the human B-cell hybridoma technique [Kozbor et al., Immunology Today, 4:72 (1983); Cote et al., Proc. Natl. Acad. Sci. U.S.A., 80:2026-2030 (1983)], and the EBV-hybridoma technique to produce human monoclonal antibodies [Cole et al., in Monoclonal Antibodies and Cancer Therapy, Alan R. Liss, Inc., pp. 77-96 (1985)]. In an additional embodiment of the invention, monoclonal antibodies can be produced in germ-free animals utilizing technology described in PCT/US90/02545. In fact, 15 according to the invention, techniques developed for the production of "chimeric antibodies" [Morrison et al., J. Bacteriol., 159:870 (1984); Neuberger et al., Nature, 312:604-608 (1984); Takeda et al., Nature, 314:452-454 (1985)] by splicing the genes from a mouse antibody molecule specific for the peptide having the amino acid 20 sequence of SEQ ID NO:3, for example, together with genes from a human antibody molecule of appropriate biological activity can be used; such antibodies are within the scope of this invention. Such human or humanized chimeric antibodies are preferred for use in therapy of human diseases or disorders (described infra), since the human or humanized antibodies are much less likely than xenogenic antibodies to induce an 25 immune response, in particular an allergic response, themselves.

According to the invention, techniques described for the production of single chain antibodies [U.S. Patent Nos. 5,476,786 and 5,132,405 to Huston; U.S. Patent 4,946,778] can be adapted to produce specific single chain antibodies. An additional embodiment of the invention utilizes the techniques described for the construction of Fab expression libraries [Huse *et al.*, *Science*, **246**:1275-1281 (1989)] to allow rapid and easy identification of monoclonal Fab fragments with the desired specificity.

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Antibody fragments which contain the idiotype of the antibody molecule can be generated by known techniques. For example, such fragments include but are not limited to: the $F(ab')_2$ fragment which can be produced by pepsin digestion of the antibody molecule; the Fab' fragments which can be generated by reducing the disulfide bridges of the $F(ab')_2$ fragment, and the Fab fragments which can be generated by treating the antibody molecule with papain and a reducing agent.

In the production of antibodies, screening for the desired antibody can be accomplished by techniques known in the art, e.g., radioimmunoassay, ELISA (enzyme-linked immunosorbant assay), "sandwich" immunoassays, immunoradiometric assays, gel diffusion precipitin reactions, immunodiffusion assays, in situ immunoassays (using colloidal gold, enzyme or radioisotope labels, for example), western blots, precipitation reactions, agglutination assays (e.g., gel agglutination assays, hemagglutination assays), complement fixation assays, immunofluorescence assays, protein A assays, and immunoelectrophoresis assays, etc. In one embodiment, antibody binding is detected by detecting a label on the primary antibody. In another embodiment, the primary antibody is detected by detecting binding of a secondary antibody or reagent to the primary antibody. In a further embodiment, the secondary antibody is labeled. Many means are known in the art for detecting binding in an immunoassay and are within the scope of the present invention. For example, to select antibodies which recognize a specific epitope of a ZA loop of a bromodomain, for example, one may assay generated hybridomas for a product which binds to a bromodomain fragment containing such an epitope and choose those which do not cross-react with bromodomain fragments that do not include that epitope.

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In a specific embodiment, antibodies that interfere with the formation of the bromodomain-acetyl-lysine complex can be generated. Such antibodies can be tested using the assays described and could potentially be used in anti-cancer therapies.

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Administration

According to the invention, the component or components of a therapeutic composition, e.g., an agent of the invention that interferes with the bromodomain-

acetyl-lysine binding complex such as the peptide having the amino acid sequence of SEQ ID NOs:4, 5, or 6 and a pharmaceutically acceptable carrier, may be introduced parenterally, transmucosally, e.g., orally, nasally, or rectally, or transdermally. Preferably, administration is parenteral, e.g., via intravenous injection, and also including, but is not limited to, intra-arteriole, intramuscular, intradermal, subcutaneous, intraperitoneal, intraventricular, and intracranial administration.

In a preferred aspect, the agent of the present invention can cross cellular and nuclear membranes, which would allow for intravenous or oral administration. Strategies are available for such crossing, including but not limited to, increasing the hydrophobic nature of a molecule; introducing the molecule as a conjugate to a carrier, such as a ligand to a specific receptor, targeted to a receptor; and the like.

The present invention also provides for conjugating targeting molecules to such an agent. "Targeting molecule" as used herein shall mean a molecule which, when administered *in vivo*, localizes to desired location(s). In various embodiments, the targeting molecule can be a peptide or protein, antibody, lectin, carbohydrate, or steroid. In one embodiment, the targeting molecule is a peptide ligand of a receptor on the target cell. In a specific embodiment, the targeting molecule is an antibody.

Preferably, the targeting molecule is a monoclonal antibody. In one embodiment, to facilitate crosslinking the antibody can be reduced to two heavy and light chain heterodimers, or the F(ab')₂ fragment can be reduced, and crosslinked to the agent via the reduced sulfhydryl. Antibodies for use as targeting molecule are specific for a cell surface antigen.

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In another embodiment, the therapeutic compound can be delivered in a vesicle, in particular a liposome [see Langer, Science, 249:1527-1533 (1990); Treat et al., in Liposomes in the Therapy of Infectious Disease and Cancer, Lopez-Berestein and Fidler (eds.), Liss: New York, pp. 353-365 (1989); Lopez-Berestein, ibid., pp. 317-327; see generally ibid.].

In yet another embodiment, the therapeutic compound can be delivered in a controlled release system. For example, the agent may be administered using intravenous

infusion, an implantable osmotic pump, a transdermal patch, liposomes, or other modes of administration. In one embodiment, a pump may be used [see Langer, supra; Sefton, CRC Crit. Ref. Biomed. Eng., 14:201 (1987); Buchwald et al., Surgery, 88:507 (1980); Saudek et al., N. Engl. J. Med., 321:574 (1989)]. In another embodiment, polymeric materials can be used [see Medical Applications of Controlled Release, Langer and Wise (eds.), CRC Press: Boca Raton, Florida (1974); Controlled Drug Bioavailability, Drug Product Design and Performance, Smolen and Ball (eds.), Wiley: New York (1984); Ranger and Peppas, J. Macromol. Sci. Rev. Macromol. Chem., 23:61 (1983); see also Levy et al., Science, 228:190 (1985); During et al., Ann. Neurol., 25:351 (1989); Howard et al., J. Neurosurg., 71:105 (1989)]. In yet another embodiment, a controlled release system can be placed in proximity of the therapeutic target, i.e., the bone marrow, thus requiring only a fraction of the systemic dose [see, e.g., Goodson, in Medical Applications of Controlled Release, supra, vol. 2, pp. 115-138 (1984)]. Other controlled release systems are discussed in the review by Langer 15 [Science, 249:1527-1533 (1990)].

Pharmaceutical Compositions. In yet another aspect of the present invention, provided are pharmaceutical compositions of the above. Such pharmaceutical compositions may be for administration for injection, or for oral, pulmonary, nasal or other forms of administration. In general, comprehended by the invention are pharmaceutical 20 compositions comprising effective amounts of a low molecular weight component or components, or derivative products, of the invention together with pharmaceutically acceptable diluents, preservatives, solubilizers, emulsifiers, adjuvants and/or carriers. Such compositions include diluents of various buffer content (e.g., Tris-HCl, acetate, 25 phosphate), pH and ionic strength; additives such as detergents and solubilizing agents (e.g., Tween 80, Polysorbate 80), anti-oxidants (e.g., ascorbic acid, sodium metabisulfite), preservatives (e.g., Thimersol, benzyl alcohol) and bulking substances (e.g., lactose, mannitol); incorporation of the material into particulate preparations of polymeric compounds such as polylactic acid, polyglycolic acid, etc. or into liposomes. 30 Hylauronic acid may also be used. Such compositions may influence the physical state, stability, rate of in vivo release, and rate of in vivo clearance of the present proteins and derivatives. See, e.g., Remington's Pharmaceutical Sciences, 18th Ed. [1990, Mack Publishing Co., Easton, PA 18042] pages 1435-1712 which are herein

incorporated by reference. The compositions may be prepared in liquid form, or may be in dried powder, such as lyophilized form.

Oral Delivery. Contemplated for use herein are oral solid dosage forms, which are described generally in Remington's Pharmaceutical Sciences, 18th Ed.1990 (Mack Publishing Co. Easton PA 18042) at Chapter 89, which is herein incorporated by reference. Solid dosage forms include tablets, capsules, pills, troches or lozenges, cachets or pellets. Also, liposomal or proteinoid encapsulation may be used to formulate the present compositions (as, for example, proteinoid microspheres reported 10 in U.S. Patent No. 4,925,673). Liposomal encapsulation may be used and the liposomes may be derivatized with various polymers (e.g., U.S. Patent No. 5,013,556). A description of possible solid dosage forms for the therapeutic is given by Marshall, K. In: Modern Pharmaceutics Edited by G.S. Banker and C.T. Rhodes Chapter 10, 1979, herein incorporated by reference. In general, the formulation will include an 15 agent of the present invention (or chemically modified forms thereof) and inert ingredients which allow for protection against the stomach environment, and release of the biologically active material in the intestine.

Also specifically contemplated are oral dosage forms of the above derivatized component or components. The component or components may be chemically modified so that oral delivery of the derivative is efficacious. Generally, the chemical modification contemplated is the attachment of at least one moiety to the component molecule itself, where said moiety permits (a) inhibition of proteolysis; and (b) uptake into the blood stream from the stomach or intestine. Also desired is the increase in overall stability of the component or components and increase in circulation time in the body. An example of such a moiety is polyethylene glycol.

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For the component (or derivative) the location of release may be the stomach, the small intestine (the duodenum, the jejunum, or the ileum), or the large intestine. One skilled in the art has available formulations which will not dissolve in the stomach, yet will release the material in the duodenum or elsewhere in the intestine. Preferably, the release will avoid the deleterious effects of the stomach environment, either by

protection of the protein (or derivative) or by release of the biologically active material beyond the stomach environment, such as in the intestine.

The therapeutic can be included in the formulation as fine multi-particulates in the form of granules or pellets of particle size about 1 mm. The formulation of the material for capsule administration could also be as a powder, lightly compressed plugs or even as tablets. The therapeutic could be prepared by compression.

One may dilute or increase the volume of the therapeutic with an inert material. These diluents could include carbohydrates, especially mannitol, a-lactose, anhydrous lactose, cellulose, sucrose, modified dextrans and starch. Certain inorganic salts may be also be used as fillers including calcium triphosphate, magnesium carbonate and sodium chloride. Some commercially available diluents are Fast-Flo, Emdex, STA-Rx 1500, Emcompress and Avicell.

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Disintegrants may be included in the formulation of the therapeutic into a solid dosage form. Materials used as disintegrates include but are not limited to starch, including the commercial disintegrant based on starch, Explotab. Binders also may be used to hold the therapeutic agent together to form a hard tablet and include materials from natural products such as acacia, tragacanth, starch and gelatin.

An anti-frictional agent may be included in the formulation of the therapeutic to prevent sticking during the formulation process. Lubricants may be used as a layer between the therapeutic and the die wall. Glidants that might improve the flow properties of the drug during formulation and to aid rearrangement during compression also might be added. The glidants may include starch, talc, pyrogenic silica and hydrated silicoaluminate.

In addition, to aid dissolution of the therapeutic into the aqueous environment a

surfactant might be added as a wetting agent. Additives which potentially enhance
uptake of the protein (or derivative) are for instance the fatty acids oleic acid, linoleic
acid and linolenic acid.

Nasal Delivery. Nasal delivery of an agent of the present invention (or derivative) is also contemplated. Nasal delivery allows the passage of a peptide, for example, to the blood stream directly after administering the therapeutic product to the nose, without the necessity for deposition of the product in the lung. Formulations for nasal delivery include those with dextran or cyclodextran.

Transdermal administration. Various and numerous methods are known in the art for transdermal administration of a drug, e.g., via a transdermal patch. Transdermal patches are described in for example, U.S. Patent No. 5,407,713, issued April 18, 1995 to Rolando et al.; U.S. Patent No. 5,352,456, issued October 4, 1004 to Fallon et al.; U.S. Patent No. 5,332,213 issued August 9, 1994 to D'Angelo et al.; U.S. Patent No. 5,336,168, issued August 9, 1994 to Sibalis; U.S. Patent No. 5,290,561, issued March 1, 1994 to Farhadieh et al.; U.S. Patent No. 5,254,346, issued October 19, 1993 to Tucker et al.; U.S. Patent No. 5,164,189, issued November 17, 1992 to Berger et al.; U.S. Patent No. 5,088,977 and 5,087,240, both issued February 18, 1992 to Sibalis; U.S. Patent No. 5,008,110, issued April 16, 1991 to Benecke et al.; and U.S. Patent No. 4,921,475, issued May 1, 1990 to Sibalis, the disclosure of each of which is incorporated herein by reference in its entirety.

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It can be readily appreciated that a transdermal route of administration may be enhanced by use of a dermal penetration enhancer, e.g., such as enhancers described in U.S. Patent No. 5,164,189 (supra), U.S. Patent No. 5,008,110 (supra), and U.S. Patent No. 4,879,119, issued November 7, 1989 to Aruga et al., the disclosure of each of which is incorporated herein by reference in its entirety.

Pulmonary Delivery. Also contemplated herein is pulmonary delivery of the pharmaceutical compositions of the present invention. A pharmaceutical composition of the present invention is delivered to the lungs of a mammal while inhaling and traverses across the lung epithelial lining to the blood stream. Other reports of this include Adjei et al. [Pharmaceutical Research, 7:565-569 (1990); Adjei et al., International Journal of Pharmaceutics, 63:135-144 (1990) (leuprolide acetate); Braquet et al., Journal of Cardiovascular Pharmacology, 13(suppl. 5):143-146 (1989)

(endothelin-1); Hubbard et al., Annals of Internal Medicine, Vol. III, pp. 206-212
(1989) (α1-antitrypsin); Smith et al., J. Clin. Invest., 84:1145-1146 (1989) (α-1-proteinase); Oswein et al., "Aerosolization of Proteins", Proceedings of Symposium on Respiratory Drug Delivery II, Keystone, Colorado, March, (1990) (recombinant human growth hormone); Debs et al., J. Immunol., 140:3482-3488 (1988) (interferon-γ and tumor necrosis factor alpha); Platz et al., U.S. Patent No. 5,284,656 (granulocyte colony stimulating factor)]. A method and composition for pulmonary delivery of drugs for systemic effect is described in U.S. Patent No. 5,451,569, issued September 19, 1995 to Wong et al.

A subject in whom administration of an agent of the present invention is an effective therapeutic regiment for cancer, for example, is preferably a human, but can be any animal. Thus, as can be readily appreciated by one of ordinary skill in the art, the methods and pharmaceutical compositions of the present invention are particularly suited to administration to any animal, e.g., for veterinary medical use, particularly for a mammal, and including, but by no means limited to, domestic animals, such as feline or canine subjects, farm animals, including bovine, equine, caprine, ovine, and porcine subjects, wild animals (whether in the wild or in a zoological garden), research animals, such as mice, rats, rabbits, goats, sheep, pigs, dogs, cats, avian species, such as chickens, turkeys, and songbirds.

The present invention may be better understood by reference to the following non-limiting Example, which is provided as exemplary of the invention. The following example is presented in order to more fully illustrate the preferred embodiments of the invention. It should in no way be construed, however, as limiting the broad scope of the invention.

EXAMPLE STRUCTURE AND LIGAND OF A HISTONE ACETYLTRANSFERASE BROMODOMAIN

Introduction

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The bromodomain is a protein motif comprising approximately 110 amino acids that is found in practically all nuclear histone acetyltransferases (HATs) [Jeanmougin et al., Trends in Biochemical Sciences, 22:151-153 (1997)]. However, despite the seemingly requisite occurrence of this motif in HATs, their role in these enzymes is unknown. Indeed, although this motif has also been identified in other chromatin proteins, heretofore not even one binding partner for a bromodomain had been identified.

Materials and Methods

Sample preparation: The bromodomain of P/CAF (residues 719-832 of SEQ ID NO:2) was subcloned into the pET14b expression vector (Novagen) and expressed in 15 Escherichia coli BL21(DE3) cells. Uniformly ¹⁵N- and ¹⁵N/¹³C-labelled proteins were prepared by growing bacteria in a minimal medium containing ¹⁵NH₄Cl with or without ¹³C₆-glucose. A uniformly ¹⁵N/¹³C-labelled and fractionally deuterated protein sample was prepared by growing the cells in 75% ²H₂O. The bromodomain was 20 purified by affinity chromatography on a nickel-IDA column (Invitrogen) followed by the removal of poly-His tag by thrombin cleavage. The final purification of the protein was achieved by size-exclusion chromatography. The acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation. NMR samples contained approximately 1 mM protein in 100mM phosphate buffer of pH 6.5 and 5mM perdeuterated DTT and $0.5 \text{ mM EDTA in H}_2\text{O}/^2\text{H}_2\text{O} (9/1) \text{ or }^2\text{H}_2\text{O}$.

NMR spectroscopy: All NMR spectra were acquired at 30°C on a Bruker DRX600 or DRX500 spectrometer. The backbone assignments of the ¹H, ¹³C, and ¹⁵N resonances 30 were achieved using deuterium-decoupled triple-resonance experiments of HNCACB and HN(CO)CACB [Yamazaki et al., J. Am. Chem. Soc. 116:11655-11666 (1994)] recorded using the uniformly ¹⁵N/¹³C-labeled and fractionally deuterated protein. The

side-chain atoms were assigned from 3D HCCH-TOCSY [Clore and Gronenborn, Meth. Enzymol. 239:249-363 (1994)] and (H)C(CO)NH-TOCSY [Logan et al., J. Biolmol. NMR 3:225-231 (1993)] data collected on the uniformly ¹⁵N/¹³C-labeled protein. Stereospecific assignments of methyl groups of the Val and Leu residues were obtained using a fractionally ¹³C-labeled sample [Neri et al., Biochemistry 28:7510-7516 (1989)]. The NOE-derived distance restraints were obtained from ¹⁵N- or ¹³C-edited 3D NOESY spectra. ϕ -angle restraints were determined based on the $^3J_{\mathrm{HN,H}}\alpha$ coupling constants measured in a 3D HNHA spectrum [Clore and Gronenborn, Meth. Enzymol. 239:249-363 (1994)]. Slowly exchanging amide protons were identified from a series of 2D ¹⁵N-HSQC spectra recorded after the H₂O buffer was changed to a ²H₂O buffer. The intermolecular NOEs used in defining the structure of the bromodomain/Ac-histamine complex were detected in ¹³C-edited (F₁), ¹³C/¹⁵N-filtered (F₃) 3D NOESY spectrum [Clore and Gronenborn, Meth. Enzymol. 239:249-363 (1994)]. All NMR spectra were processed with the NMRPipe/NMRDraw 15 programs and analyzed using NMRView [Johnson and Blevins, J. Biomol., NMR 4:603-614 (1994)].

Structure calculations: Structures of the bromodomain were calculated with a distance geometry/simulated annealing protocol using the X-PLOR program [Brunger, A. X-20 PLOR Version 3.1: A system for X-Ray crystallography and NMR, Yale University Press, New Haven, CT, (1993)]. A total of 1324 manually assigned NOE-derived distance restraints were obtained from the ¹⁵N- and ¹³C-edited NOE spectra. Further analysis of the NOE spectra was carried out by the iterative automated assignment procedure using ARIA [Nilges and O'Donoghue, Prog. NMR Spectroscopy 32:107-139 25 (1998)], which integrates with X-PLOR for structure calculations. A total of 1519 unambiguous and 590 ambiguous distance restraints were identified from the NOE data by ARIA, many of which were checked and confirmed manually. The ARIA-assigned distance restraints were in agreement with the structures calculated using only the manually assigned NOE distance restraints, 28 hydrogen-bond distance restraints for 14 hydrogen bonds, and 54 ϕ -angle restraints. The final structure 30 calculations employed a total of 3515 NMR experimental restraints obtained from the manual and the ARIA-assisted assignments, 2843 of which were unambiguously assigned NOE-derived distance restraints that comprise of 1077 intra-residue, 621

sequential, 550 medium-range, and 595 long-range NOEs. For the ensemble of the final 30 structures, no distance and torsional angle restraints were violated by more than 0.3\AA and 5° , respectively. The total, distance violation, and dihedral violation energies were 178.7 ± 2.4 kcal mol⁻¹, 41.6 ± 0.9 kcal mol⁻¹, and 0.50 ± 0.06 kcal mol⁻¹, respectively. The Lennard-Jones potential which was not used during any refinement stage, was -526.2 ± 16.8 kcal mol⁻¹ for the final structures. Ramachandran plot analysis of the final structures (residues 727-828) with Procheck-NMR [Laskowski *et al.*, *J. Biolmol. NMR* 8:477-486 (1996)] showed that $71.0 \pm 0.6\%$, $23.8 \pm 0.6\%$, $3.5 \pm 0.2\%$, and $1.7 \pm 0.2\%$ of the non-Gly and non-Pro residues were in the most favorable, additionally allowed, generously allowed, and disallowed regions, respectively. The corresponding values for the residues in the four α -helices (residues 727-743, 770-776, 785-802, and 807-827) were $88.9 \pm 0.4\%$, $11.0 \pm 0.4\%$, $0.1 \pm 0.1\%$, and $0.0 \pm 0.0\%$, respectively. The structure of the bromodomain/acetyl-histamine complex was determined using the free form structure and additional 25 intermolecular and 5 intra-ligand NOE-derived distance restraints.

Site-directed mutagenesis: Mutant proteins were prepared using the QuickChange site-directed mutagenesis kit (Stratagene). The presence of appropriate mutations was confirmed by DNA sequencing.

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Ligand titration: Ligand titration experiments were performed by recording a series of 2D ¹⁵N- and ¹³C-HSQC spectra on the uniformly ¹⁵N-, and ¹⁵N/¹³C-labelled bromodomain (~0.3mM), respectively, in the presence of different amounts of ligand concentration ranging from 0 to approximately 2.0 mM. The protein sample and the stock solutions of the ligands were all prepared in the same aqueous buffer containing 100mM phosphate and 5mM perdeuterated DTT at pH 6.5.

The full length nucleic acid sequence of the human p300/CBP-associated factor (P/CAF) was obtained from GenBank. Accession No: U57317.2 (SEQ ID NO:1):

30 1 gg
61 gg

1 ggggccgcgt cgacgcggaa aagaggccgt ggggggcctc ccagcgctgg cagacaccgt
61 gaggctggca gccgcggca cgcacaccta gtccgcagtc ccgaggaaca tgtccgcagc
121 cagggcgcgg agcagagtcc cgggcaggag aaccaaggga gggcgtgtgc tgtggcggcg
181 gcggcagcgg cagcggagcc gctagtcccc tcccttgg gggagcagct gccgccgctg
241 ccgccgccgc caccaccatc agcggcggg gcccggccag agcgagccgg gcgagcggg

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301 cgctaggggg agggcggggg cggggagggg ggtgggcgaa gggggggga gggcgtgggg
           361 ggagggtete getetecega etaceagage eegagggaga eeetggegge ggeggeggeg
           421 cctgacactc ggcgcctcct gccgtgctcc ggggcggcat gtccgaggct ggcggggccg
           481 ggccgggcgg ctgcggggca ggagccgggg caggggccgg gcccgggggcg ctgcccccgc
 5
           541 ageotgegge getteegeee gegeeeeege agggeteeee etgegeeget geegeegggg
           601 getegggege etgeggteeg gegaeggeag tggetgeage gggeaeggee gaaggaeegg
           661 gaggeggtgg eteggeeega ategeegtga agaaagegea aetaegetee geteegeggg
           721 ccaagaaact ggagaaactc ggagtgtact ccgcctgcaa ggccgaggag tcttgtaaat
           781 gtaatggctg gaaaaaccct aacccctcac ccactccccc cagagccgac ctgcagcaaa
10
           841 taattgtcag tctaacagaa tcctgtcgga gttgtagcca tgccctagct gctcatgttt
           901 cccacctgga gaatgtgtca gaggaagaaa tgaacagact cctgggaata gtattggatg
           961 tggaatatct ctttacctgt gtccacaagg aagaagatgc agataccaaa caagtttatt
          1021 tctatctatt taagctcttg agaaagtcta ttttacaaag aggaaaacct gtggttgaag
          1081 gctctttgga aaagaaaccc ccatttgaaa aacctagcat tgaacagggt gtgaataact
15
          1141 ttgtgcagta caaatttagt cacctgccag caaaagaaag gcaaacaata gttgagttgq
          1201 caaaaatgtt cctaaaccgc atcaactatt ggcatctgga ggcaccatct caacgaagac
          1261 tgcgatctcc caatgatgat atttctggat acaaagagaa ctacacaagg tggctgtgtt
          1321 actgcaacgt gccacagttc tgcgacagtc tacctcggta cgaaaccaca caggtgtttg
          1381 ggagaacatt gcttcgctcg gtcttcactg ttatgaggcg acaactcctg gaacaagcaa
20
          1441 gacaggaaaa agataaactg cctcttgaaa aacgaactct aatcctcact catttcccaa
          1501 aatttctgtc catgctagaa gaagaagtat atagtcaaaa ctctcccatc tgggatcagg
          1561 attttctctc agcctcttcc agaaccagcc agctaggcat ccaaacagtt atcaatccac
          1621 ctcctgtggc tgggacaatt tcatacaatt caacctcatc ttcccttgag cagccaaacg
          1681 cagggagcag cagtcctgcc tgcaaagcct cttctggact tgaggcaaac ccaggagaaa
25
          1741 agaggaaaat gactgattct catgttctgg aggaggccaa gaaaccccga gttatggggg
         1801 atattccgat ggaattaatc aacgaggtta tgtctaccat cacggaccct gcagcaatgc
          1861 ttggaccaga gaccaatttt ctgtcagcac actcggccag ggatgaggcg gcaaggttgg
         1921 aagagcgcag gggtgtaatt gaatttcacg tggttggcaa ttccctcaac cagaaaccaa
         1981 acaagaagat cctgatgtgg ctggttggcc tacagaacgt tttctcccac cagctgcccc
30
         2041 gaatgccaaa agaatacatc acacggctcg tctttgaccc gaaacacaaa accettgctt
         2101 taattaaaga tggccgtgtt attggtggta tctgtttccg tatgttccca tctcaaggat
         2161 tcacagagat tgtcttctgt gctgtaacct caaatgagca agtcaagggc tatggaacac
         2221 acctgatgaa tcatttgaaa gaatatcaca taaagcatga catcctgaac ttcctcacat
         2281 atgcagatga atatgcaatt ggatacttta agaaacaggg tttctccaaa gaaattaaaa
35
         2341 tacctaaaac caaatatgtt ggctatatca aggattatga aggagccact ttáatgggat
         2401 gtgagctaaa tccacggatc ccgtacacag aattttctgt catcattaaa aagcagaagg
         2461 agataattaa aaaactgatt gaaagaaaac aggcacaaat tcgaaaagtt taccctggac
         2521 tttcatgttt taaagatgga gttcgacaga ttcctataga aagcattcct ggaattagag
         2581 agacaggetg gaaacegagt ggaaaagaga aaagtaaaga geecagagae eetgaecage
40
         2641 tttacagcac gctcaagagc atcctccagc aggtgaagag ccatcaaagc gcttggccct
         2701 tcatggaacc tgtgaagaga acagaagctc caggatatta tgaagttata aggttcccca
         2761 tggatctgaa aaccatgagt gaacgcctca agaataggta ctacgtgtct aagaaattat
         2821 tcatggcaga cttacagcga gtctttacca attgcaaaga gtacaacgcc gctgagagtg
         2881 aatactacaa atgtgccaat atcctggaga aattcttctt cagtaaaatt aaggaagctg
```

2941 gattaattga caagtgattt tttttccccc tctgcttctt agaaactcac caagcagtgt 3001 gcctaaagca aggt

The full length protein sequence of the human p300/CBP-associated factor (P/CAF)

- 5 was obtained from GenBank. Accession No: U57317.2, (SEQ ID NO:2):
 - MSEAGGAGPG GCGAGAGAGA GPGALPPQPA ALPPAPPQGS PCAAAAGGSG ACGPATAVAA
 - 61 AGTAEGPGGG GSARIAVKKA QLRSAPRAKK LEKLGVYSAC KAEESCKCNG WKNPNPSPTP
 - 121 PRADLQQIIV SLTESCRSCS HALAAHVSHL ENVSEEEMNR LLGIVLDVEY LFTCVHKEED
 - 181 ADTKQVYFYL FKLLRKSILQ RGKPVVEGSL EKKPPFEKPS IEQGVNNFVQ YKFSHLPAKE
- 10 241 RQTIVELAKM FLNRINYWHL EAPSQRRLRS PNDDISGYKE NYTRWLCYCN VPQFCDSLPR
 - 301 YETTQVFGRT LLRSVFTVMR RQLLEQARQE KDKLPLEKRT LILTHFPKFL SMLEEEVYSQ
 - 361 NSPIWDQDFL SASSRTSQLG IQTVINPPPV AGTISYNSTS SSLEQPNAGS SSPACKASSG
 - 421 LEANPGEKRK MTDSHVLEEA KKPRVMGDIP MELINEVMST ITDPAAMLGP ETNFLSAHSA
 - 481 RDEAARLEER RGVIEFHVVG NSLNQKPNKK ILMWLVGLQN VFSHQLPRMP KEYITRLVFD
- 15 541 PKHKTLALIK DGRVIGGICF RMFPSQGFTE IVFCAVTSNE QVKGYGTHLM NHLKEYHIKH
 - 601 DILNFLTYAD EYAIGYFKKQ GFSKEIKIPK TKYVGYIKDY EGATLMGCEL NPRIPYTEFS
 - 661 VIIKKQKEII KKLIERKQAQ IRKVYPGLSC FKDGVRQIPI ESIPGIRETG WKPSGKEKSK
 - 721 EPRDPDQLYS TLKSILQQVK SHQSAWPFME PVKRTEAPGY YEVIRFPMDL KTMSERLKNR
 - 781 YYVSKKLFMA DLQRVFTNCK EYNAAESEYY KCANILEKFF FSKIKEAGLI DK

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Results

The P/CAF bromodomain represents an extensive family of bromodomains (Figure 1). A large number of long-range nuclear Overhauser enhancement (NOE)-derived

25 distance restraints were identified in the NMR data of the P/CAF bromodomain, yielding a well-defined three-dimensional structure (Figures 2A -2D). Table 1 shows the NMR chemical shift assignment of the P/CAF bromodomain. Table 2 shows the Unambiguous NOE-derived distance restraints. Table 3 shows the Ambiguous NOE-derived distance restraints. Table 4 shows the Hydrogen bond restraints. The NMR structure coordinates of the P/CAF bromodomain in the free and complexed to acetyl-histamine are shown in Tables 5 and 6, respectively.

The structure consists of a four-helix bundle (helices α_Z , α_A , α_B , and α_C) with a left-handed twist, and a long intervening loop between helices α_Z and α_A (termed the ZA loop, Figure 2E). The four amphipathic α -helices are packed tightly against one another in an antiparallel manner, with crossing angles for adjacent helices of ~16-20°. The up-and-down four-helix bundle can adapt two topological folds with opposite

handedness (Figures 2F-2G). The right-handed four-helix bundle fold occurs more commonly and is seen in proteins such as hemerythrin and cytochrome b_{562} . The left-handed fold of the bromodomain structure is less common, but also observed in proteins such as cytochrome b₅ and T4 lysozyme [Richardson, J., Adv. Protein Chem., 34:167-339 (1989); Presnell and Cohen, Proc. Natl. Acad. Sci. USA 86:6592-6596 (1989)]. This topological difference arises from the orientation of the loop between the first two helices (Fig. 2F-2G). The right-handed four-helix bundle proteins have a relatively short hairpin-like connection between the first two helices, which makes the "preferred" turn to the right at the top of the first helix [Richardson, J., Adv. Protein Chem., 34:167-339 (1989); Presnell and Cohen, Proc. Natl. Acad. Sci. USA 86:6592-6596 (1989); Weber and Salemme, Nature 287:82-84 (1980)]. In contrast, proteins with the left-handed fold usually have a long loop after the first helix and often contain additional secondary structural elements at the base of the helix bundle [Richardson, J., Adv. Protein Chem., 34:167-339 (1989); Presnell and Cohen, Proc. Natl. Acad. Sci. USA 86:6592-6596 (1989)]. In the bromodomain structure, this long ZA loop has a defined conformation and is packed against the loop between helices α_B and α_C (termed the BC loop) to form a hydrophobic pocket. These tertiary interactions between the two loops appear to favor the left turn of the ZA loop, resulting in the left-handed four-helix bundle fold of the bromodomain. The hydrophobic pocket formed by loops 20 ZA and BC is lined by residues Val752, Ala757, Tyr760, Val763, Tyr802 and Tyr809 (Fig. 2H), and appears to be a site for protein-protein interactions (see below). The pocket is located at one end of the four-helix bundle, opposite to the N- and C-termini of the protein. Interestingly, the ZA loop varies in length amongst different bromodomains, but almost always contains residues corresponding to Phe748, Pro751, Pro758, Tyr760, and Pro767 (Figure 1). The conservation of these residues within the 25 ZA loop as well as residues within the α-helical regions implies a similar left-handed four-helix bundle structure for the large family of bromodomains (Fig. 1).

The modular bromodomain structure supports the idea that bromodomain can act as a functional unit for protein-protein interactions. The observation that bromodomains are found in nearly all known nuclear HATs (A-type) that are known to promote transcription-related acetylation of histones on specific lysine residues, but not present in cytoplasmic HATs (B-type), prompted the determination of whether bromodomains

can interact with acetyl-lysine (AcK). The NMR titration of the P/CAF bromodomain were performed with a peptide (SGRGKGG-AcK-GLGK) derived from histone H4, in which Lys8 is acetylated (Lys8 is the major acetylation site in H4 for GCN5, a yeast homologue of P/CAF). Remarkably, the bromodomain could indeed bind the AcK peptide. Moreover, this interaction appeared to be specific, based on the ¹⁵N-HSOC spectra which showed that only a limited number of residues underwent chemical shift changes as a function of peptide concentration (Figure 3A). Conversely, the NMR titration of the bromodomain with a non-acetylated, but otherwise identical H4 peptide. showed no noticeable chemical shift changes, demonstrating that the interaction 10 between the bromodomain and the lysine-acetylated H4 peptide was dependent upon acetylation of lysine. The dissociation constant (K_D) for the AcK peptide was estimated to be $346 \pm 54 \mu M$. This binding is likely reinforced through additional interactions between bromodomain-containing proteins and target proteins. Notably, many chromatin-associated proteins contain two or multiple bromodomains (Figure 1). Indeed, binding with another lysine-acetylated peptide (RKSTGG-AcK-APRKQ) 15 derived from the major acetylation site on histone H3 (residues 9-20) was also observed. Together, these data demonstrate that the P/CAF bromodomain has the ability to bind AcK peptides in an acetylation dependent manner.

Intriguingly, the bromodomain residues that exhibited the most significant ¹H and ¹⁵N 20 chemical shift changes on peptide binding are located near the hydrophobic pocket between the ZA and BC loops (Figure 3B). Because a similar pattern of amide chemical shift changes was observed with the two different AcK-containing peptides, it was surmised that the hydrophobic cavity is the primary binding site for AcK. This 25 hypothesis was further supported by titration with acetyl-histamine, which mimics the chemical structure of the AcK side-chain (Figure 3C). Both ¹⁵N- and ¹³C-HSOC spectra showed that interaction with acetyl-histamine was also acetylation-dependent, involving the same set of residues that showed chemical shift perturbations with similar concentration dependence. It should be noted that the bromodomain did not 30 bind to the amino acids acetyl-lysine or acetyl-histidine alone, possibly due to the presence of the charged amino, carboxyl, or caboxylate group adjacent to the acetyl moiety (Figure 3C). Taken together, these results strongly suggest that the P/CAF

bromodomain can interact with acetyl-lysine-containing proteins in a specific manner, and that this interaction is localized to the bromodomain hydrophobic cavity.

To identify the key residues involved in bromodomain-AcK recognition, the NMR structure of the P/CAF bromodomain in complex with acetyl-histamine was elucidated. As anticipated, the acetylated moiety binds in the bromodomain hydrophobic pocket (Figure 4). The intermolecular interactions are largely hydrophobic in nature, with the methyl group of acetyl-histamine making extensive contacts with the side-chains of Val752, Ala757, and Tyr760, and the methylene groups of acetyl-histamine displaying specific NOEs to Val752, Ala757, Tyr760, Tyr802, and Tyr809. No intermolecular NOEs were observed for the imidazole ring of acetyl-histamine. From the spectral analysis it is clear that the structure of the bromodomain is very similar in both the free and complex forms.

- It is worth noting that the bromodomain-AcK recognition is reminiscent of the interactions between the histone acetyltransferase Hat1 and acetyl-CoA. Although the binding pockets of these two otherwise structurally unrelated proteins are composed of different secondary structural elements, the nature of acetyl-lysine recognition has striking similarities. In particular, Tyr809, Tyr802, Tyr760, and Val752 in the bromodomain appear to be related to Phe220, Phe261, Val254, and Ile217 of Hat1, respectively, in their interactions with the acetyl moiety. This observation may suggest an evolutionary convergent mechanism of acetyl-lysine recognition between bromodomains and histone acetyltransferases.
- To determine the relative contributions of residues within the hydrophobic cavity in bromodomain-AcK binding, site-directed mutagenesis was used to alter residues Tyr809, Tyr802, Tyr760, and Val752 (Table 7).

Table 7. Structural and Functional Analysis of the P/CAF Bromodomain Mutants

5	Bromodomain Proteins	Structural Integrity ^a	H4 AcK-Peptide Binding $K_{ m D}(\mu{ m M})^{ m b}$
	Wild-Type	++++	346 ± 54
10	Tyr809Ala	++++	No Binding ^c
	Tyr802Ala	+++	> 10,000 ^d
	Tyr760Ala	+++	> 10,000
15	Val752Ala	++	> 10,000

- a. The effects of mutations on the structural integrity of the bromodomain were assessed by using the ¹⁵N-HSQC spectra. The amide ¹H/¹⁵N resonances of the mutant proteins were compared to those of the wild-type bromodomain to determine if the particular mutations lead to global or local structure disruption. Severe line-broadening of the amide resonances would indicate protein conformational exchange due to a decrease of structure stability resulting from point mutations. Structural integrity of the mutant proteins is expressed here relative to that of the wild-type, using the signs of "++++" for as stable as the wild-type, "+++" for mildly destabilized, "++" for moderately destabilized, and "-" for completely unfolded.
- b. The ligand binding affinity (K_D) of the bromodomain proteins was estimated by following chemical shift changes of amide peaks in the ¹⁵N-HSQC spectra as a
 function of the ligand concentration.
 - c. No detectable ligand binding observed in the NMR titration.
- d. Ligand binding affinity was significantly reduced and beyond the limit for reliable
 measurements by NMR titration.

Substitution of Ala for Tyr809 completely abrogated the bromodomain binding to the lysine-acetylated H4 peptide, while the Tyr802Ala, Tyr760Ala, and Val752Ala mutants had significantly reduced ligand binding affinity. To assess whether these mutations disrupted the overall bromodomain fold, the ¹⁵N-HSOC spectra of the mutants was compared to that of the wild-type protein. For the Tyr809Ala mutant, the amide chemical shifts were only affected for a few residues near the mutation site. However, mutations of the other residues in the hydrophobic binding pocket perturbed the local protein conformation to greater extents, particularly the ZA loop (Table 7). Thus, the NMR structural analysis and the mutagenesis studies show that Tyr809, which is structurally supported by Trp746 and Asn803 (Fiure 4), is essential for the bromodomain interaction with the acetyl group of acetyl-lysine, while residues of Tyr802, Tyr760, and Val752 likely play both structural and functional roles in the recognition. These residues are highly conserved throughout the bromodomain family (Figure 1), suggesting that recognition of acetyl-lysine may be a feature of bromodomains, in general. Therefore, Val752, Ala757, Tyr760, Tyr802, Asn803, and 15 Tyr809 are key amino acid residues for the P/CAF bromodomain binding to acetyllysine.

Table 8: Amino Acid Sequences of Bromodomains Identified in Figure 1

		T	1	1		
	PROTEIN	SEQ ID	GenBank	PROTEIN	SEQ ID	GenBank
	BD	NO:	Acc. No.	BD	NO:	Acc. No.
	hsp/CAF	7	U57317	dmFSH-2	25	
5	hsGCN5	8	U57136	scBDF1-2	26	
	ttP55	9	U47321	hsBR140	27	JC2069
	scGCN5	10	Q03330	hsSMAP	28	X87613
	hsP300	11	A54277	ggPB1-1	29	X90849
	hsCBP	12	S39162	ggPB1-2	30	
10	mmCBP	13	S39161	ggPB1-3	31	
	ceYNJ1	14	P34545	ggPB1-4	32	
	hsCCG1-1	15	P21675	ggPB1-5	33	
	msCCG1-1	16	D26114	spBRO-1	34	S54260
	hsCCG1-2	17		spBRO-2	35	
15	msCCG1-2	18		hsSNF2a	36	S45251
	hsRing3-1	19	P25440	hsBRG1	37	S39039
	hsORFX-1	20	D26362	ggBRM	38	X91638
	dmFSH-1	21	P13709	ggBRG1	39	X91637
	scBDF1-1	22	P35817	hsTIF1b	40	X97548
20	hsRing3-2	23		mmTIF1b	41	X99644
	hsORFX-2	24		mmTIF1a	42	S78219

The present invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description and the accompanying figures. Such modifications are intended to fall within the scope of the appended claims.

It is further to be understood that all base sizes or amino acid sizes, and all molecular weight or molecular mass values, given for nucleic acids or polypeptides are approximate, and are provided for description.

5 Various publications are cited herein, the disclosures of which are hereby incorporated by reference herein in their entireties.

Table 1	HETEROGENEITY 100	CA 62.320000	CG1 28.733000
	N 121.192000	HA 4.038000	HG11 1.748000
	HN 8.416000	CB 38.640000	HG12 1.052000
	CA 63.430000	HB1 3.211000	CG2 17.168000
NMR Chemical Shift Assignment	HA 4.331000 CB 30.930000 HB1 1.815000	HB2 3.024000 CD1 134.350000	HG2# 1.003000 CD1 13.863000
of the P/CAF	HB1 1.815000 HB2 1.762000 CG 27.630000	HD1 7.053000 CE1 119.481000	HD1# 0.619000 END_RES_DEP
Bromodomain	HG1 1.681000 CD 43.603000	HE1 6.882000 END_RES_DBF	RES_ID 736
	HD1 3.161000 END_RES_DEF	RES_ID 730 RES_TYPE SER	RES_TYPE LEU SPIN_SYSTEM_ID 22 HETEROGENBITY 100
RES_ID 715	RES_ID 724	SPIN SYSTEM ID 16	N 119.880000
RES_TYPE GLY		HETEROGENEITY 100	HN 8.841000
SPIN_SYSTEM_ID 1	RES_TYPE ASP	N 112.173000	CA 58.473000
HETEROGENEITY 100	SPIN_SYSTEM_ID 10	HN 8.167000	HA 4.090000
END_RES_DEF	HETEROGENEITY 100	HA 3.920000	CB 41.950000
	N 122.012000	HB1 3.995000	HB1 2.090000
RES_ID 716 RES_TYPE SER SPIN_SYSTEM_ID 2	HN 8.273000 CA 52.415000	END_RES_DEF	HB2 1.703000 CG 27.330000
HETEROGENEITY 100	HA 4.874000	RES_ID 731 RES_TYPE THR	HG 1.759000
END_RES_DEF	CB 41.400000		CD1 26.530000
RES_ID 717	HB1 2.754000 HB2 2.692000 END_RES_DEF	SPIN_SYSTEM_ID 17 HETEROGENEITY 100 N 120.372000	HD1# 1.061000 CD2 23.776000
RES_TYPE HIS	RES_ID 725	HN 8.059000	HD2# 0.977000
SPIN_SYSTEM_ID 3		CA 66.730000	END_RES_DEF
HETEROGENEITY 100	RES_TYPE PRO	HA 3.924000	RES_ID 737
END_RES_DEP	SPIN_SYSTEM_ID 11	CB 68.930000	RES_TYPE GLN
RES_ID 718	HETEROGENEITY 100	КВ 4.247000	SPIN SYSTEM ID 23
	CA 65.080000	CG2 21.570000	HETEROGENEITY 100
RES_TYPE MET SPIN_SYSTEM_ID 4	HA 4.329000	HG2# 1.142000	N 117.256000
	CB 32.590000	END_RES_DEF	HN 8.505000
HETEROGENEITY 100	HB1 2.326000	RES_ID 732	CA 59.020000
END_RES_DEP	HB2 1.973000		HA 4.032000
RES_ID 719 RES_TYPE SER	CG 27.632000 HG1 2.028000 CD 51.310000	RES_TYPE LEU SPIN_SYSTEM_ID 18 HETEROGENEITY 100	CB 28.182000 HB1 2.327000 HB2 2.263000
SPIN_SYSTEM_ID 5	HD1 3.866000	N 120.536000	CG 34.240000
HETEROGENEITY 100	END_RES_DEF	HN 8.460000	HG1 2.536000
END_RES_DEF	RES_ID 726	CA 57.920000 HA 3.289000	HG2 2.461000 END_RES_DEF
RES_ID 720	RES_TYPE ASP	CB 39.750000	RES_ID 738
RES_TYPE LYS	SPIN_SYSTEM_ID 12	HB1 1.532000	
SPIN_SYSTEM_ID 6	HETEROGENEITY 100	HB2 0.294000	RES_TYPE GLN
HETEROGENEITY 100	N 119.716000	CG 24.880000	SPIN_SYSTEM_ID 24,7
CA 56.296000 HA 4.361000 CB 33.140000	HN 8.397000 CA 55.720000	HG 1.683000 CD1 25.429000	HETEROGENEITY 100 N 118.896000
HB1 1.882000 HB2 1.684000	HA 4.692000 CB 40.550000 HB1 2.792000	HD1# 0.469000 CD2 19.921000 HD2# -0.193000	HN 8.033000 CA 59.574000 HA 4.196000
CG 25.430000	HB2 2.730000	END_RES_DEF	CB 29.835000
HG1 1.585000	END_RES_DEF		HB1 2.482000
HG2 1.433000	RES_ID 727	RES_ID 733	HB2 2.469000
CD 29.834000		RES_TYPE LYS	CG 35.342000
HD1 1.703000	RES_TYPE GLN SPIN_SYSTEM_ID 13	SPIN_SYSTEM_ID 19	HG1 2.840000
CE 41.960000		HETEROGENEITY 100	HG2 2.467000
HE1 3.003000 END_RES_DEF	HETEROGENEITY 100 N 121.356000 HN 8.196000	N 118.568000 HN 8.563000	NE2 110.369000 HE21 7.022000
ES_ID 721 ES_TYPE GLU	CA 55.920000 HA 4.163000	CA 60.125000 HA 3.679000 CB 32.588000	HE22 6.916000 END_RES_DEP
SPIN_SYSTEM_ID 7	CB 28.730000	HB1 1.729000	RES_ID 739 RES_TYPE VAL
SETEROGENEITY 100	HB1 2.148000	HB2 1.360000	
N 122.990000	CG 34.240000	CG 24.880000	SPIN_SYSTEM_ID . 25
HN 8.317000	HG1 2.524000	HG1 1.280000	HETEROGENEITY 100
CA 54.620000	HG2 2.371000	CD 29.835000	N 119.716000
HA 4.540000	END_RES_DEF	HD1 1.585000	HN 8.526000
CB 29.830000 HB1 2.024000 HB2 1.893000	RES_ID 728	CB 41.960000 HE1 2.918000	CA 67.830000 HA 3.844000
CG 35.893000 HG1 2.271000	RES_TYPE LEU SPIN_SYSTEM_ID 14 HETEROGENEITY 100	END_RES_DEF RES_ID 734	CB 32.030000 HB 2.384000
ND_RES_DEF	N 121.356000 HN 8.210000	RES_ID 734 RES_TYPE SER SPIN_SYSTEM_ID 20	CG1 23.330000 HG1# 1.183000 CG2 22.120000
ES_ID 722	CA 58.473000	HETEROGENEITY 100	HG2# 1.033000
ES_TYPE PRO	HA 4.045000	N 113.157000	END_RES_DEF
PIN_SYSTEM_ID 8	CB 41.400000	HN 7.540000	RES_ID 740
ETEROGENEITY 100	HB1 1.847000	CA 61.227000	
CA 63.430000	HB2 1.555000	HA 4.281000	RES_TYPE LYS
HA 4.393000	CG 27.080000	CB 63.879000	SPIN_SYSTEM_ID 26
CB 32.030000	HG 1.480000	HB1 4.060000	HETEROGENEITY 100
HB1 2.224000	CD1 25.970000	END_RES_DEF	N 114.633000
HB2 1.880000 CG 27.630000 HG1 2.028000	HD1# 0.794000 CD2 23.226000	RES_ID 735	HN 8.572000 CA 59.574000
CD 50.760000 HD2 3.656000	HD2# 0.786000 END_RES_DEF	RES_TYPE ILE SPIN_SYSTEM_ID 21 HETEROGENEITY 100	HA 3.886000 CB 32.380000 HB1 1.873000
HD1 3.800000	RES_ID 729 RES_TYPE TYR	N 120.700000	HG1 1.022000
ND_RES_DEF		HN 7.951000	HD1 1.520000
ES_ID 723	SPIN_SYSTEM_ID 15 HETEROGENEITY 100	CA 65.080000 HA 3.786000	END_RES_DEP
ES_TYPE ARG	N 119.060000	CB 38.095000	RES_ID 741
PIN_SYSTEM_ID 9	HN 8.021000	HB 1.879000	RES_TYPE SER

SPIN_SYSTEM_ID 27 HETEROGENEITY 100			
	RES_TYPE PRO	END_RES_DEF	CB 39.750000
N 110.369000	SPIN_SYSTEM_ID 33		HB1 2.689000
HN 7.557000	HETEROGENEITY 100	RES_ID 753	HB2 2.487000
CA 59.024000	CA 64.531000 HA 3.756000	RES_TYPE LYS	CD1 133.799000
HA 4.448000		SPIN_SYSTEM_ID 39	HD1 5.120000
CB 63.980000	CB 29.835000 HB1 0.487000	HETEROGENEITY 100	CE1 118.379000
HB1 4.004000	HB2 -0.783000	N 129.883000	HE1 6.070000
END_RES_DEF	CG 26.53000	HN 9.045000	end_res_dep
	HG1 0.233000	CA 56.310000 HA 4.370000	
RES_ID 742	HG2 -0.931000	CB 32.880000	RES_ID 761
RES_TYPE HIS	CD 50.212000	HB1 1.873000	RES_TYPE TYR
SPIN_SYSTEM_ID 28	HD2 1.567000	HG1 1.435000	SPIN_SYSTEM_ID 47
HETEROGENEITY 100	HD1 2.177000	HD1 1.673000	HETEROGENEITY 100
N 125.619000	END_RES_DEF	HE1 2.985000	N 113.157000
HN 7.536000		END RES DEF	HN 8.225000
CA 58.473000	RES_ID 748		CA 60.676000
HA 3.967000	RES_TYPE PHE	RES_ID 754	HA 4.101000 CB 37.550000
CB 32.588000	SPIN_SYSTEM_ID 34	RES_TYPE ARG	
HB1 2.990000	HETEROGENEITY 100	SPIN_SYSTEM_ID 40	HB1 3.189000 HB2 2.801000
HB2 2.799000	N 113.321000	HETEROGENEITY 100	CD1 134.901000
CD2 118.930000	HN 7.585000	N 120.208000	HD1 7.342000
HD2 4.978000	CA 55.719000	HN 8.054000	CE1 118.930000
CE1 138.755000	HA 4.930000	END_RES_DEF	HE1 6.646000
HE1 7.522000	CB 39.202000	· · · · · · · · · · · · · · · · ·	END_RES_DEP
END_RES_DEP	. HB1 3.491000	RES ID 755	okao_bar
	HB2 2.532000	RES_TYPE THR	RES_ID 762
RES_ID 743	CD1 133.248000	SPIN_SYSTEM_ID 41	RES_TYPE GLU
RES_TYPE GLN	HD1 7.099000	HETEROGENEITY 100	SPIN SYSTEM ID 48
SPIN_SYSTEM_ID 29	HE1 7.174000	CA 63.430000	HETEROGENEITY 100
HETEROGENEITY 100	HZ 7.296000	HA 4.038000	N 117.912000
N 128.571000	END_RES_DEF	CB 68.380000	HN 7.702000
HN 8.543000		HB 4.293000	CA 57.922000
CA 59.125000	RES_ID 749	CG2 22.670000	HA 4.209000
HA 4.209000	RES_TYPE MET	HG2# 1.267000	CB 29.480000
CB 29.834000	SPIN_SYSTEM_ID 35	END_RES_DEF	HB1 2.086000
HB1 2.111000	HETEROGENEITY 100		CG 37.545000
CG 33.690000	N 117.748000	RES_ID 756	HG1 2.325000
HG1 2.390000	HN 7.115000	RES_TYPE GLU	HG2 2.265000
NE2 112.173000	CA 56.820000	SPIN_SYSTEM_ID 42	END_RES_DEF
HE21 7.581000	HA 4.286000	HETEROGENEITY 100	
HE22 6.870000	CB 32.590000	N 118.732000	RES_ID 763
end_res_def	HB1 2.233000	HN 7.209000	RES_TYPE VAL
RES_ID 744	HB2 2.174000	CA 56.270000	SPIN_SYSTEM_ID 49
RES_TYPE SER	CG 33.140000	HA 4.448000	HETEROGENEITY 100
SPIN_SYSTEM_ID 30	HG1 2.851000	CB 30.930000	N 115.453000
HETEROGENEITY 100	CE 17.168000	HB1 2.174000	HN 7.135000
N 119.060000	HE# 2.175000	HB2 2.000000	CA 63.430000
HN 11.668000	END_RES_DEF	CG 36.440000	HA 4.077000
CA 60.125000	RES ID 750	HG1 2.292000	CB 33.690000
HA 4.838000	_ _	END_RES_DEF	HB 2.015000
CB 63.980000	RES_TYPE GLU . SPIN_SYSTEM_ID 36	200 10 200	CG1 21.020000
		RES_ID 757	HG1# 1.045000
101 9.334UUU			
HB1 4.334000 HB2 3.926000		RES_TYPE ALA	CG2 21.574000
HB2 3.926000	N 113.813000	SPIN_SYSTEM_ID 43	HG2# 0.991000
	N 113.813000 HN 7.709000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100	
HB2 3.926000	N 113.813000 HN 7.709000 CA 53.516000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000	HG2# 0.991000 END_RES_DEF
HB2 3.926000 END_RES_DEF	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000	HG2# 0.991000 END_RES_DEF RES_ID 764
HB2 3.926000 END_RES_DEF RES_ID 745	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEP	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HETEROGENEITY 100	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEP RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN SYSTEM ID 37 HETEROGENEITY 100 CA 62.879000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEP RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETERGGENBITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HETEROGENEITY 100 CA 62.879000 HA 4.242000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000 CB 31.447000	HGC# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HGI1 0.798000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEP RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HHTEROGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.370000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000 CB 31.487000 HB1 2.374000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000
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HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 CA 73.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HA 4.368000 CA 60.691000 HA 4.368000 CB 27.630000 HB1 3.594000 HB1 3.594000 HB1 3.594000 HB1 3.594000 HB1 7.897000 NEI 110.861000 CD1 128.843000 HD1 7.897000 NEI 110.474000 CC3 122.234000 HE3 7.336000 CC22 116.177000 HC2 7.382000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN SYSTEM ID 37 HETEROGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB1 2.328000 HB1 2.16000 HG1 2.196000 CG 27.080000 HG1 2.196000 CG 27.080000 HG1 3.670000 CD 50.763000 HD1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN SYSTEM ID 38 HETEROGENEITY 100 N 124.450000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000 CB 31.487000 HB1 2.374000 HB2 2.027000 CG 27.632000 HG2 2.038000 CD 50.212000 HG1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HSTEROGENEITY 100 END_RES_DEF	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETEROGENEITY 100 N 125.291000 HN 7.749000 CA 57.371000 HA 3.875000 CB 30.936000 HB1 1.388000 HB2 1.211000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HB 4 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HN 7.135000 CA 60.691000 HA 4.368000 CB 27.630000 HB1 3.594000 HB2 3.351000 CD1 128.843000 HD1 7.897000 NEI 110.861000 HB1 10.474000 CE3 122.234000 HB3 7.3366000 CC2 116.177000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HSTERGGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB2 1.683000 CG 27.080000 HG1 2.126000 HG2 1.978000 CD 50.763000 HG1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN_SYSTEM_ID 38 HETERGGENEITY 100 N 124.450000 HN 8.1244000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CB 31.487000 HB1 2.374000 HB1 2.374000 HB1 2.374000 HG1 2.122000 HG2 2.038000 CD 50.212000 HG2 2.038000 CD 50.212000 HD1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETEROGENEITY 100 HN 7.749000 CA 57.371000 HN 7.749000 CA 57.371000 HN 7.749000 CA 57.371000 HA 3.875000 CB 30.936000 HB1 1.388000 HB2 1.211000 CC 27.080000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HA 4.368000 CA 60.691000 HA 4.368000 CB 27.630000 HB1 3.594000 HB2 3.351000 CD1 128.843000 HD1 7.897000 NEI 110.861000 HB1 10.474000 CC3 122.234000 HE3 7.336000 CC2 116.177000 HC2 7.382000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HHETERGGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB1 2.328000 HB1 2.328000 HG2 1.683000 CG 27.080000 CG 27.080000 HG1 2.126000 HG2 1.978000 CD 50.763000 HG1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN_SYSTEM_ID 38 HETERGGENEITY 100 N 124.450000 HN 8.124000 CA 63.430000 CC 53.430000 CC A 63.430000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000 CB 31.487000 HB1 2.374000 HB2 2.027000 CG 27.632000 HG2 2.038000 CD 50.212000 HG2 2.038000 CD 50.212000 HD1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF RES_ID 760 RES_DEF	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETTERCGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETERCGENEITY 100 N 125.291000 HN 7.749000 CA 57.371000 HA 3.875000 CB 30.936000 HB1 1.388000 HB2 1.211000 CG 27.080000 HG1 1.319000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HA 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HA 4.368000 CA 60.691000 HA 4.368000 CB 27.630000 HB1 3.594000 HB1 3.594000 HB1 3.594000 HB1 7.897000 NEI 110.861000 HB1 17.897000 NEI 110.474000 CC3 122.234000 HE3 7.336000 CC22 116.177000 HC2 7.382000 CC23 123.336000 HC3 7.197000 CC3 122.334000 HC3 7.390000 CC3 123.336000 HC3 7.197000 CC3 122.334000 HC3 7.390000 CC3 123.336000 HC3 7.197000 CC3 126.089000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN SYSTEM_ID 37 HETEROGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB2 1.683000 CG 27.080000 HG1 2.126000 HG1 2.126000 HG1 2.196000 HG1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN SYSTEM_ID 38 HETEROGENEITY 100 N 124.450000 HN 8.124000 CA 63.430000 HA 3.553000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000 CB 31.487000 HB1 2.374000 HB2 2.027000 CG 27.632000 HG1 2.132000 HG2 2.038000 CD 50.212000 HG2 3.515000 HD1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF RES_ID 760 RES_TYPE TYR SPIN_SYSTEM_ID 46	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETEROGENEITY 100 N 125.291000 CA 57.371000 HN 7.749000 CA 57.371000 CB 30.936000 HB1 1.388000 HB2 1.211000 CG 27.0800000 HG1 1.319000 HG2 1.319000 HG2 1.319000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HN 7.135000 CA 60.691000 HA 4.368000 CB 27.630000 HB1 3.594000 HB2 3.351000 CD1 128.843000 HD1 7.897000 NEI 110.861000 HD1 7.897000 NEI 110.861000 HD2 7.336000 CZ2 116.177000 HC2 7.382000 CZ2 123.336000 HZ3 7.197000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HSTERGGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB2 1.683000 CG 27.080000 HG1 2.126000 HG2 1.978000 CD 50.763000 HG1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN_SYSTEM_ID 38 HETERGGENEITY 100 N 124.450000 HN 8.124000 CA 63.430000 HN 8.124000 CA 63.430000 CA 63.430000 CA 63.430000 CA 33.553000 CB 32.580000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 56.080000 HA 4.496000 CB 31.487000 HB1 2.374000 HB2 2.027000 CG 27.632000 HG2 2.038000 CD 50.212000 HG2 2.038000 CD 50.212000 HG1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETEROGENEITY 100 HN 7.749000 CA 57.371000 HN 7.749000 CA 57.371000 HA 3.875000 CB 30.936000 HB1 1.388000 HB2 1.211000 CG 27.080000 HG1 1.319000 CG 27.080000 HG1 1.319000 CC 41.052000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HA 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HA 4.368000 CA 60.691000 HA 4.368000 CB 27.630000 HB1 3.594000 HB1 3.594000 HB1 3.594000 HB1 7.897000 NEI 110.861000 HB1 17.897000 NEI 110.474000 CC3 122.234000 HE3 7.336000 CC22 116.177000 HC2 7.382000 CC23 123.336000 HC3 7.197000 CC3 122.334000 HC3 7.390000 CC3 123.336000 HC3 7.197000 CC3 122.334000 HC3 7.390000 CC3 123.336000 HC3 7.197000 CC3 126.089000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HETEROGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB1 2.328000 HB1 2.328000 HG2 1.683000 CG 27.080000 HG2 1.978000 CD 50.763000 HG1 2.126000 HG2 1.978000 CD 50.763000 HD1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN_SYSTEM_ID 38 HETEROGENEITY 100 N 124.450000 HN 8.124000 CA 63.430000 HA 3.553000 CB 32.580000 HA 3.553000 CB 32.580000 HB 1.145000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000 CB 31.487000 HB1 2.374000 HB2 2.027000 CG 27.632000 HG1 2.122000 HG2 2.038000 CD 50.212000 HG2 3.515000 HD1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 RES_TYPE TYR SPIN_SYSTEM_ID 45 HETEROGENEITY 100 RES_TYPE TYR SPIN_SYSTEM_ID 46 HETEROGENEITY 100 N 122.504000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETERCGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETERCGENEITY 100 N 125.291000 HN 7.749000 CA 57.371000 HA 3.875000 CB 30.936000 HB1 1.388000 HB2 1.211000 CG 27.080000 HG1 1.319000 HG2 1.173000 CD 43.052000 HG1 1.319000 HG1 1.319000 HG2 1.173000 CD 43.052000 HD1 2.971000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HA 4.368000 CA 60.691000 HA 4.368000 CB 27.630000 HB1 3.594000 HB2 3.351000 CD1 128.843000 HD1 7.897000 NEI 110.841000 CE3 122.234000 HE1 10.474000 CE3 122.234000 HE2 7.336000 CZ2 116.177000 HZ2 7.382000 CZ2 116.177000 HZ2 7.382000 CZ2 123.336000 HZ3 7.197000 CH2 126.089000 HH2 7.150000 END_RES_DEF	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN SYSTEM_ID 37 HETEROGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB2 1.683000 CG 27.080000 HG1 2.126000 HG1 2.126000 HG1 2.196000 HG1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN SYSTEM_ID 38 HETEROGENEITY 100 N 124.450000 HN 8.124000 CA 63.430000 HN 8.124000 CA 63.430000 HN 8.124000 CA 63.430000 CB 32.580000 HB 1.1450000 CG 27.580000 CB 32.580000 CG 32.580000 CG 31.573000 CG 21.573000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 HB# 1.082000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 56.080000 HA 4.496000 CB 31.487000 HB1 2.374000 HB2 2.027000 CG 27.632000 HG2 2.038000 CD 50.212000 HG2 2.038000 CD 50.212000 HG1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HETEROGENEITY 100 END_RES_DEF	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETEROGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETEROGENEITY 100 HN 7.749000 CA 57.371000 HN 7.749000 CA 57.371000 HA 3.875000 CB 30.936000 HB1 1.388000 HB2 1.211000 CG 27.080000 HG1 1.319000 CG 27.080000 HG1 1.319000 CC 41.052000
HB2 3.926000 END_RES_DEF RES_ID 745 RES_TYPE ALA SPIN_SYSTEM_ID 31 HETEROGENEITY 100 N 117.584000 HN 7.868000 CA 53.510000 HA 4.396000 CB 20.470000 HB# 1.688000 END_RES_DEF RES_ID 746 RES_TYPE TRP SPIN_SYSTEM_ID 32 HETEROGENEITY 100 N 116.600000 HN 7.135000 CA 60.691000 HA 4.368000 CB 27.630000 HB2 3.351000 CD 128.843000 HB1 3.594000 HB2 3.351000 CD1 128.843000 HB1 10.474000 CE3 122.234000 HE1 10.474000 CE3 122.234000 HE2 7.382000 CC2 116.177000 HC2 7.3820000 CC2 126.089000 HC2 7.150000	N 113.813000 HN 7.709000 CA 53.516000 HA 4.849000 CB 31.487000 HB1 2.091000 HB2 1.730000 CG 35.893000 HG1 2.164000 END_RES_DEF RES_ID 751 RES_TYPE PRO SPIN_SYSTEM_ID 37 HSTERGGENEITY 100 CA 62.879000 HA 4.242000 CB 32.040000 HB1 2.328000 HB2 1.683000 CG 27.080000 HG1 2.166000 HG2 1.978000 CD 50.763000 HG1 3.670000 END_RES_DEF RES_ID 752 RES_TYPE VAL SPIN_SYSTEM_ID 38 HETERGGENEITY 100 N 124.450000 HN 8.124000 CA 63.430000 HA 3.553000 CB 32.580000 HB 1.145000 CG 21.573000 CG 21.573000 CG 22.580000 HB 1.145000 CG 22.580000 HB 1.145000 CG 21.573000	SPIN_SYSTEM_ID 43 HETEROGENEITY 100 N 122.504000 HN 7.379000 CA 50.220000 HA 4.937000 CB 19.370000 END_RES_DEF RES_ID 758 RES_TYPE PRO SPIN_SYSTEM_ID 44 HETEROGENEITY 100 CA 65.080000 HA 4.496000 CB 31.487000 HB1 2.374000 HB2 2.027000 CG 27.632000 HG1 2.132000 HG2 2.038000 CD 50.212000 HG1 3.717000 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HSTEROGENEITY 100 END_RES_DEF RES_ID 759 RES_TYPE GLY SPIN_SYSTEM_ID 45 HSTEROGENEITY 100 END_RES_DEF RES_ID 760 RES_TYPE TYR SPIN_SYSTEM_ID 46 HSTEROGENEITY 100 END_RES_TYPE TYR SPIN_SYSTEM_ID 46 HSTEROGENEITY 100 N 122.504000 HN 7.945000	HG2# 0.991000 END_RES_DEF RES_ID 764 RES_TYPE ILE SPIN_SYSTEM_ID 50 HETERCGENEITY 100 N 122.832000 HN 7.947000 CA 57.920000 HA 3.916000 CB 34.240000 HB 1.205000 CG1 24.878000 HG11 0.798000 HG12 0.216000 CG2 16.617000 HG2# 0.380000 CD1 9.457000 HD1# 0.537000 END_RES_DEF RES_ID 765 RES_TYPE ARG SPIN_SYSTEM_ID 51 HETERCGENEITY 100 N 125.291000 HN 7.749000 CA 57.371000 HA 3.875000 CB 30.936000 HB1 1.388000 HB2 1.211000 CG 27.080000 HG1 1.319000 HG2 1.173000 CD 43.052000 HG1 1.319000 HG1 1.319000 HG2 1.173000 CD 43.052000 HD1 2.971000

RES_TYPE SER SPIN_SYSTEM_ID 52			
SPIN SYSTEM IN S2	END_RES_DEP	CD1 25.429000	SPIN_SYSTEM_ID 69
		HD1# 1.067000	HETEROGENEITY 100
HETEROGENEITY 100	RES ID 772	CD2 27.081000	N 115.780000
N 116.600000	RES TYPE THR		
		HD2# 0.871000	HN 7.698000
HN 8.387000	SPIN_SYSTEM_ID 58	end_res_def	CA 62.330000
CA 54.618000	HETEROGENEITY 100		HA 4.083000
HA 4.984000	N 122.176000	RES ID 778	CB 31.500000
CB 38.640000	HN 9.445000	RES TYPE LYS	HB 2.321000
HB1 3.034000	CA 67.040000	SPIN_SYSTEM_ID 64	CG1 21.570000
HB2 2.907000	HA 3.845000		
		HETEROGENEITY 100	HG1# 0.944000
END_RES_DEP	CB 67.835000	N 120.372000	CG2 18.820000
	HB 4.090000	HN 7.958000	HG2# 0.823000
RES_ID 767	CG2 22.124000	CA 59.574000	END_RES_DEF
RES_TYPE PRO	HG2# 1.058000	HA 4.333000	<u>-</u> ···-
SPIN SYSTEM ID 53	END_RES_DEF	CB 32.588000	DEC 10 004
	mp_kg2_pgt		RES_ID 784
		HB1 2.055000	res_type ser
CA 63.429000	RES_ID 773	CG 24.878000	SPIN_SYSTEM_ID 70
HA 4.083000	RES_TYPE MET	HG1 1.596000	HETEROGENEITY 100
CB 32.588000	SPIN_SYSTEM_ID 59	CD 29.835000	N 111.353000
HB1 2.209000	HETEROGENEITY 100	HD1 1.804000	HN 7.415000
CG 28.180000			
	N 117.912000	CE 41.951000	CA 55.719000
HG1 2.177000	HN 7.882000	HE1 2.990000	HA 4.741000
HG2 1.883000	CA 60.676000	end_res_def	CB 66.183000
°CD 50.763000	HA 4.319000		HB1 4.200000
HD2 3.390000	CB 33.342000	RES_ID 779	HB2 3.750000
HD1 3.623000	HB1 2.093000	RES TYPE ASN	
			END_RES_DEF
END_RES_DEF	HB2 1.915000	SPIN_SYSTEM_ID 65	
	CG 33.139000	HETEROGENEITY 100	RES_ID 785
RES_ID 768	HG1 2.621000	N 116.108000	RES_TYPE LYS
RES_TYPE MET	HG2 2.496000	HN 7.947000	SPIN SYSTEM ID 71
SPIN SYSTEM ID 54	CE 16.620000	CA 53.510000	HETEROGENEITY 100
	HE# 1.241000	HA 4.771000	CA 59.030000
N 119.060000	end_res_def	CB 38.095000	HA 4.021000
HN 8.430000		HB1 3.019000	CB 31.590000
CA 54.067000	RES ID 774	HB2 2.773000	END_RES_DEF
HA 4.935000	RES TYPE SER	ND2 112.665000	· ·
CB 31.487000	SPIN SYSTEM ID 60		222 12 206
		HD21 7.598000	RES_ID 786
HB1 1.989000	HETEROGENEITY 100	HD22 6.969000	RES_TYPE LYS
HB2 1.353000	N 116.108000	END_RES_DEF	SPIN_SYSTEM_ID 72
CG 30.930000	HN 7.958000		HETEROGENEITY 100
HG1 2.690000	CA 62.879000	RES ID 780	N 120.208000
CE 14.414000	HA 4.200000	RES_TYPE ARG	HN 8.244000
HE# 1.929000	CB 62.879000	SPIN SYSTEM ID 66	CA 59.720000
END_RES_DEF	HB1 4.368000	HETEROGENEITY 100	HA 4.062000
222	HB2 4.040000		
RES ID 769		N 114.141000	CB 30.385000
	END_RES_DEF	HN 8.158000	HB1 1.779000
RES_TYPE ASP		CA 56.821000	متے CG 24.530000
SPIN_SYSTEM_ID 55	RES_ID 775	HA 4.405000	CD 28.182000
HETEROGENEITY 100	RES_TYPE GLU	CB 25.429000	HD1 1.680000
N 119.060000	SPIN SYSTEM ID 61	HB1 2.097000	CE 41.670000
HN 7.365000	HETEROGENEITY 100	HB2 2.022000	HE1 3.137000
CA 53.516000	N 124.471000	CG 27.632000	
CA 53.516000	N 124.471000	CG 27.632000	HE2 3.045000
HA 4.745000	HN 8.150000	HG1 1.539000	END_RES_DEF
HA 4.745000 CB 44.154000	HN 8.150000 CA 59.570000	HG1 1.539000 HG2 1.534000	END_RES_DEF
HA 4.745000	HN 8.150000	HG1 1.539000	
HA 4.745000 CB 44.154000	HN 8.150000 CA 59.570000	HG1 1.539000 HG2 1.534000	END_RES_DEF RES_ID 787
HA 4.745000 CB 44.154000 HB1 2.371000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000	END_RES_DEF RES_ID 787 RES_TYPE LEU
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETERGENEITY 100 N 118.732000 HN 7.422000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETEROGENEITY 100	HN 8.150000 CA 59.57000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56	HN 8.150000 CA 59.57000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETERGENEITY 100 N 118.732000 HN 7.422000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETEROGENEITY 100	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETEROGENEITY 100 N 116.272000 HN 9.055000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 END_RES_DEP	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN SYSTEM ID 67 HETEROGENEITY 100	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETEROGEMEITY 100 HN 9.055000 CA 57.922000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176600 END_RES_DEP RES_ID 776	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETERGGENEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 END_RES_DEP RES_ID 776 RES_TYPE ARG	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000 HBI 1.996000 HBI 1.996000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETEROGENEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE SPIN_SYSTEM_ID 56 HETEROGEMEITY 100 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176600 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE SPIN SYSTEM_ID 56 HETEROGEMEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB2 1.395000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100 N 120.372000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE SPIN_SYSTEM_ID 56 HETEROGEMEITY 100 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176600 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE SPIN SYSTEM_ID 56 HETEROGEMEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB2 1.395000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100 N 120.372000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.924000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HTTERGGEMEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 HB2 1.395000 HG 1.713000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176600 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100 H 120.372000 HN 8.391000 CA 60.676000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB2 2.055000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.924000 CD2 23.776000
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HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETEROGENEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 HB1 2.095000 HG 1.713000 CD 27.080000 HD1# 0.940000	HN 8.150000 CA 59.57000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG2 2.345000 HG2 2.176000 END_RES_DEF RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100 N 120.372000 HN 8.191000 CA 60.676000 HA 3.869000 CB 30.385000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETERCGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB2 2.055000 CD1 134.350000 HD1 6.2850000 HD1 6.285000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.924000 CD2 23.776000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE SPIN_SYSTEM_ID 56 HETEROGEMEITY 100 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 CG 27.080000 HG 1.713000 CD1 27.080000 HG 1.713000 CD1 27.080000 HG 1.713000 CD2 22.675000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176600 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100 HN 8.391000 CA 60.676000 HA 3.869000 CB 30.385000 HB1 2.047000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DDF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB2 2.055000 CD1 134.350000 HD1 6.285000 CD1 134.350000 HD1 6.285000 CE1 118.930000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 CA 57.922000 CA 57.922000 CA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.924000 CD2 23.776000 HD2# 0.895000 END_RES_DEF
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE LEU SPIN_SYSTEM_ID 56 HETEROGENEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 HB1 2.095000 HG 1.713000 CD 27.080000 HD1# 0.940000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 END_RES_DEF RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HHETEROGENEITY 100 M 120.372000 HN 8.191000 CA 60.676000 HA 3.869000 CB 30.385000 HB1 2.047000 HB2 1.076000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETERCGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB2 2.055000 CD1 134.350000 HD1 6.2850000 HD1 6.285000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.924000 CD2 23.776000 HD2# 0.895000
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE SPIN_SYSTEM_ID 56 HETEROGEMEITY 100 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 CG 27.080000 HG 1.713000 CD1 27.080000 HG 1.713000 CD1 27.080000 HG 1.713000 CD2 22.675000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176600 END_RES_DEP RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100 HN 8.391000 CA 60.676000 HA 3.869000 CB 30.385000 HB1 2.047000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD2 3.024000 END_RES_DDF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB2 2.055000 CD1 134.350000 HD1 6.285000 CD1 134.350000 HD1 6.285000 CE1 118.930000	END_RES_DEF RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 CA 57.922000 CA 57.922000 CA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.924000 CD2 23.776000 HD2# 0.895000 END_RES_DEF
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HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE 56 HETEROGENEITY 100 N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 HB2 1.395000 CG 27.080000 HG1 7.713000 CD1 27.080000 HD1# 0.940000 CD2 22.675000 HD1# 0.628000 END_RES_DEF RES_ID 771 RES_TYPE LYS SPIN_SYSTEM_ID 57 HETEROGENEITY 100 N 128.079000 HN 8.738000 CA 60.676600 HA 4.198000 CB 32.037000 HB1 2.330000 HB2 2.224000 CG 25.280000 HG2 1.403000 CG 30.385000 HG1 1.403000 CG 30.385000 HG1 1.403000 CG 30.385000 HG1 1.793000	HN 8.150000 CA 59.57000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG2 2.345000 HG2 2.176000 EMD_RES_DEF RES_ID 776 RES_TYPE ARG SPIN_SYSTEM_ID 62 HETEROGENEITY 100 HN 8.191000 CA 60.676000 HA 8.391000 CB 30.385000 HB1 2.047000 HB1 2.047000 HB2 1.076000 CC 29.284000 HG1 1.722000 HG2 0.877000 CD 44.154000 HD1 2.578000 EMD_RES_DEF RES_ID 777 RES_TYPE LEU SPIN_SYSTEM_ID 63 HETEROGENEITY 100 HC2 2.081000 HC3 1.722000 HC4 1.54000 HC5 1.777 RC5_TYPE LEU SPIN_SYSTEM_ID 63 HETEROGENEITY 100 N 120.208000 HN 8.865000 CA 58.470000 HA 4.691000 CB 42.621000 HC5 2.295000 HC6 42.621000 HC7 42.621000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD1 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB1 2.948000 HB1 6.285000 CD1 134.350000 CD1 134.350000 HD1 6.285000 CD1 134.350000 HD1 6.285000 CD1 134.350000 HD1 6.285000 CD1 134.350000 HD1 6.3850000 CD1 133.248000 HD1 3.0620000 HD2 2.9070000 CD1 133.248000 HD1 7.1750000 CD1 133.248000 HD1 7.1750000 CE1 120.582000	RES_ID 787 RES_TYPE 100 RES_TYPE 100 RES_TYSTEM_ID 73 RETEROGENEITY 100 N 118.732000 HN 7.422000 CA 57.922000 HA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.9799000 HD1# 0.924000 CD2 23.776000 HD2# 0.895000 EMD_RES_DEF RES_ID 788 RES_TYPE PHE SPIN_SYSTEM_ID 74 HETEROGENEITY 100 N 118.732000 HN 6.928000 CA 60.676000 HA 3.761000 CB 39.750000 HB1 2.945000 HB1 2.945000 HB1 2.945000 HB1 2.945000 HB1 2.945000 HB1 6.928000 CD1 133.799000 HD1 6.400000 CE1 131.596000 HE1 6.928000 EMD_RES_DEF RES_ID 789 RES_TYPE MET
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE 56 HHTEROGEMEITY N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 HG 1.713000 CD1 27.080000 HG 1.713000 CD2 22.675000 HD1# 0.940000 CD2 22.675000 HD1# 0.940000 CD2 22.675000 HD1# 0.940000 CD2 17.080000 HD1# 0.940000 CD3 22.675000 HD1# 0.940000 CD4 17.080000 HD1# 0.940000 CD5 18.095000 HD1# 0.940000 CD6 19.095000 HD1# 0.940000 CD7 19.095000 HD1# 0.940000 CD8 19.095000 HD1# 0.711 CD8 19.095000 HD1# 0.711 CD8 19.095000 HD1# 0.712 CD9 19.095000 HD1# 0.712 CD 19.095000 HD1# 0.712 CD 10.095000 HD1 1.795000 HD1 1.795000 HD1 1.795000 HD2 1.6956000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 EMD_RES_DEF RES_ID 776 RES_TYPE 3PIN SYSTEM_ID 62 HETEROGENEITY 100 M 120.372000 HM 8.391000 CA 60.676000 HA 3.869000 CB 30.385000 HB1 2.047000 HB2 1.076000 CG 29.284000 HG2 1.722000 HG2 2.051000 EMD_RES_DEF RES_ID 777 RES_TYPE LEU SPIN SYSTEM_ID 63 HETEROGENEITY 100 HD1 2.578000 HD2 2.051000 EMD_RES_DEF RES_ID 777 RES_TYPE LEU SPIN SYSTEM_ID 663 HETEROGENEITY 100 N 120.208000 HM 8.856000 CA 58.470000 HA 4.691000 CB 42.621000 HB1 2.295000 HB2 1.295000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB1 2.948000 HB1 6.285000 CD1 134.350000 CD1 134.350000 HD1 6.2850000 END_RES_DEF RES_ID 782 RES_TYPE TYR SPIN_SYSTEM_ID 68 HETEROGENEITY 100 N 114.633000 HN 8.014000 CA 57.920000 HA 4.528000 CB 36.443000 HB1 3.0620000 HB1 3.0620000 HB1 3.0620000 HB1 2.9977000 CD1 133.248000 HD1 7.175000 CCE1 120.582000 HE1 7.286000 END_RES_DEF	RES_ID 787 RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETERGGENEITY 100 N 118.732000 CA 57.922000 CA 57.922000 CA 42.13000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.9924000 CD2 23.776000 HD2# 0.895000 END_RES_DEF RES_ID 788 RES_TYPE PHE SPIN_SYSTEM_ID 74 HETERGGENEITY 100 N 118.732000 CA 60.676000 HA 3.763000 CB 39.750000 HB1 2.945000 CB 39.750000 HB1 2.945000 CB 133.799000 HD1 6.928000 CC 1 133.799000 HD1 6.400000 CEI 131.596000 HE1 6.928000 END_RES_DEF RES_ID 789 RES_TYPE MET SPIN_SYSTEM_ID 75
HA 4.745000 CB 44.15400 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE SPIN_SYSTEM_ID 5100 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 CG 27.080000 HB1 2.095000 CG 27.080000 HG 1.713000 CD1 27.080000 HG 1.713000 END_RES_DEF RES_ID 771 RES_TYPE LYS SPIN_SYSTEM_ID 57 HETEROGENEITY 100 N 128.079000 HN 8.738000 CA 60.676000 HA 4.198000 CB 32.037000 HB1 2.330000 HB1 1.483000 CC 25.280000 HG2 1.403000 CC 30.385000 HD1 1.793000 HD2 1.696000 CC 41.9550000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176600 END_RES_DEP RES_ID 776 RES_TYPE SPIN_SYSTEM_ID 62 HETEROGENEITY 100 N 120.372000 HN 8.391000 CA 60.6766000 HA 3.869000 CB 30.385000 HB1 2.047000 HB2 1.076000 CG 29.284000 HG2 0.877000 CD 44.154000 HG1 1.722000 HG2 0.877000 CD 44.154000 HD1 2.578000 HD2 2.051000 END_RES_DEF RES_ID 777 RES_TYPE LEU SPIN_SYSTEM_ID 63 HETEROGENEITY 100 HR 1.020000 HR 8.856000 CA 58.470000 HA 4.691000 CG 42.621000 HB1 2.295000 HB2 1.925000 CG 27.080000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HAA 4.064000 CB 40.850000 HB1 2.948000 HB1 2.948000 HB1 2.948000 HB1 2.955000 CD1 134.350000 HD1 6.285000 CE1 118.930000 HD1 6.709000 END_RES_DEF RES_ID 782 RES_TYPE TYR SPIN_SYSTEM_ID 68 HETEROGENEITY 100 N 114.633000 HN 8.014000 CA 57.920000 HA 4.528000 HA 4.528000 CB 36.443000 HB1 3.062000 HB2 2.997000 CD1 133.248000 HD1 7.175000 CE1 120.582000 HE1 7.286000 END_RES_DEF	RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETEROGENEITY 100 N 118.732000 CA 57.922000 CA 57.922000 CA 4.213000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.924000 CD2 23.776000 HD2# 0.895000 END_RES_DEF RES_ID 788 RES_TYPE PHE SPIN_SYSTEM_ID 74 HETEROGENEITY 100 N 118.732000 HA 3.761000 CA 60.676000 HA 3.761000 CB 39.750000 HB1 2.945000 CB 39.750000 CB
HA 4.745000 CB 44.154000 HB1 2.371000 END_RES_DEF RES_ID 770 RES_TYPE 56 HHTEROGEMEITY N 116.272000 HN 9.055000 CA 57.922000 HA 4.036000 CB 41.400000 HB1 2.095000 HG 1.713000 CD1 27.080000 HG 1.713000 CD2 22.675000 HD1# 0.940000 CD2 22.675000 HD1# 0.940000 CD2 22.675000 HD1# 0.940000 CD2 17.080000 HD1# 0.940000 CD3 22.675000 HD1# 0.940000 CD4 17.080000 HD1# 0.940000 CD5 18.095000 HD1# 0.940000 CD6 19.095000 HD1# 0.940000 CD7 19.095000 HD1# 0.940000 CD8 19.095000 HD1# 0.711 CD8 19.095000 HD1# 0.711 CD8 19.095000 HD1# 0.712 CD9 19.095000 HD1# 0.712 CD 19.095000 HD1# 0.712 CD 10.095000 HD1 1.795000 HD1 1.795000 HD1 1.795000 HD2 1.6956000	HN 8.150000 CA 59.570000 HA 4.045000 CB 29.280000 HB1 2.246000 HB2 2.063000 CG 36.443000 HG1 2.345000 HG2 2.176000 EMD_RES_DEF RES_ID 776 RES_TYPE 3PIN SYSTEM_ID 62 HETEROGENEITY 100 M 120.372000 HM 8.391000 CA 60.676000 HA 3.869000 CB 30.385000 HB1 2.047000 HB2 1.076000 CG 29.284000 HG2 1.722000 HG2 2.051000 EMD_RES_DEF RES_ID 777 RES_TYPE LEU SPIN SYSTEM_ID 63 HETEROGENEITY 100 HD1 2.578000 HD2 2.051000 EMD_RES_DEF RES_ID 777 RES_TYPE LEU SPIN SYSTEM_ID 663 HETEROGENEITY 100 N 120.208000 HM 8.856000 CA 58.470000 HA 4.691000 CB 42.621000 HB1 2.295000 HB2 1.295000	HG1 1.539000 HG2 1.534000 CD 43.050000 HD1 3.060000 HD1 3.060000 HD2 3.024000 END_RES_DEF RES_ID 781 RES_TYPE TYR SPIN_SYSTEM_ID 67 HETEROGENEITY 100 N 116.764000 HN 8.222000 CA 60.125000 HA 4.064000 CB 40.850000 HB1 2.948000 HB1 2.948000 HB1 6.285000 CD1 134.350000 CD1 134.350000 HD1 6.2850000 END_RES_DEF RES_ID 782 RES_TYPE TYR SPIN_SYSTEM_ID 68 HETEROGENEITY 100 N 114.633000 HN 8.014000 CA 57.920000 HA 4.528000 CB 36.443000 HB1 3.0620000 HB1 3.0620000 HB1 3.0620000 HB1 2.9977000 CD1 133.248000 HD1 7.175000 CCE1 120.582000 HE1 7.286000 END_RES_DEF	RES_ID 787 RES_ID 787 RES_TYPE LEU SPIN_SYSTEM_ID 73 HETERGGENEITY 100 N 118.732000 CA 57.922000 CA 57.922000 CA 42.13000 CB 43.603000 HB1 1.996000 HB2 1.891000 CG 27.632000 HG 1.794000 CD1 25.979000 HD1# 0.9924000 CD2 23.776000 HD2# 0.895000 END_RES_DEF RES_ID 788 RES_TYPE PHE SPIN_SYSTEM_ID 74 HETERGGENEITY 100 N 118.732000 CA 60.676000 HA 3.763000 CB 39.750000 HB1 2.945000 CB 39.750000 HB1 2.945000 CB 133.799000 HD1 6.928000 CC 1 133.799000 HD1 6.400000 CEI 131.596000 HE1 6.928000 END_RES_DEF RES_ID 789 RES_TYPE MET SPIN_SYSTEM_ID 75

HN 8.48900		HETEROGENEITY	100	HETEROGENE ITY	100	SPIN SYSTEM_I	D 94
CA 59.0200		N 117.9120	00	N 117.91200		HETEROGENEITY	
HA 3.91100		HN 7.013000)	HN 7.945000		N 123.4880	
CB 32.5900		CA 66.73000		CA 57.99200	0	HN 9.06100	
HB1 2.3180		HA 3.039000)	HA 4.250000		CA 59.57400	
HB2 2.2080		CB 30.93000		CB 30.38500	0	HA 4.232000	0
CG 33.1400		HB 1.435000		HB1 2.17200		CB 29.83500	00
HG1 2.9420		CG1 22.1240		HB2 2.00300		HB1 2.16900	00
HG2 2.6110		HG1# 0.4790		CG 36.99400		CG 36.44300	00
CE 17.1680		CG2 21.5730		HG1 2.40700		HG1 2.52800	00
HE# 2.02700	0	HG2# 0.1420	100	HG2 2.20300	0	END_RES_DEF	
end_res_def		end_res_def		end_res_def			
RES_ID	790	200 10			***	RES_ID	809
RES TYPE	ALA	RES_ID RES_TYPE	796 PHE	RES_ID	802	RES_TYPE	TYR
SPIN SYSTEM II		SPIN_SYSTEM ID		RES_TYPE	TYR	SPIN_SYSTEM_ID	
HETEROGENEITY	100	HETEROGENE ITY	100	SPIN_SYSTEM_ID HETEROGENEITY		HETEROGENEITY	100
N 119.71600		N 116.92800		N 116.60000	100	N 116.43600	
HN 8.000000		HN 6.357000			9	HN 8.072000	
CA 55.17000		CA 58.47000		HN 7.744000 CA 60.67600		CA 60.12000	
HA 4.084000		HA 4.161000		CA 60.67600 HA 4.369000	•	HA 3.834000	
CB 18.27000		CB 38.09600		CB 41.40000	,	CB 37.55000	
HB# 1.48500		HB1 3.09000		HB1 2.92900		HB1 3.01800	
END RES DEF		HB2 2.94400		CD1 134.901		HB2 2.73800	
		CD1 132.147		HD1 6.98900		CD1 132.698 HD1 6.89100	
RES ID	791	HD1 6.64100		CE1 119.481		HD1 6.89100 CE1 120.032	
RES_TYPE	ASP	CE1 131.596		HE1 6.823000		HE1 7.01100	
SPIN SYSTEM ID	77	HE1 6.45600		END_RES_DEF		END_RES_DEF	U
HETEROGENEITY	100	CZ 129.3930				m40_KB3_DEF	
N 119.71600	0	HZ 6.406000		RES_ID	803	RES ID	810
HN 7-376000		END RES DEF		RES TYPE	ASN	RES_TYPE	TYR
CA 57.37100	0			SPIN SYSTEM ID	89	SPIN SYSTEM ID	
HA 4.371000		RES_ID	797	HETEROGENEITY	100	HETEROGENEITY	100
CB 38.64600	0	RES_TYPE	THR	N 115.944000		N 119.88000	
HB1 2.73000	0	SPIN_SYSTEM_ID	83	HN 8.241000		HN 7.356000	-
END_RES_DEF		HETEROGENEITY	100	CA 51.864000		CA 61.777000	0
		N 115.289000		HA 5.024000		HA 3.819000	-
RES_ID	792	HN 9.047000		CB 40.849000		CB 40.30000	0
RES_TYPE	LEU	CA 66.734000)	HB1 3.069000		HB1 3.390000	
SPIN_SYSTEM_ID	78	HA 3.838000		HB2 2.907000		HB2 2.500000	
heterogene I ty	100	CB 68.380000)	ND2 118.7320	00	CD1 136.5530	
N 119.55000	0	HB 4.210000		HD21 8.31600	0	HD1 7.094000	
HN 7.363000	_	CG2 22.12000		HD22 7.80900	0	CE1 119.4810	000
CA 57.92200	9	HG2# 1.29600	00	END_RES_DEF		HE1 7.000000	0
HA 3.398000		END_RES_DEP				END_RES_DEF	
CB 40.299000				RES_ID	804		
HB1 0.757000		RES_ID	798	RES_TYPE	ALA	RES_ID	812
HB2 0.442000 CG 27.632000		RES_TYPE	ASN	SPIN_SYSTEM_ID	90	RES_TYPE	LYS
	,	SPIN_SYSTEM_ID	84	HETEROGENE ITY	100	SPIN_SYSTEM_ID	97
HG 0.707000		HETEROGENEITY	100	END_RES_DEF		HETEROGENEITY	100
CD1 24.32700 HD1# 0.18400		N 120.700000				N 118.076000)
CD2 25.97900		HN 8.846000		RES_ID	805	HN 8.072000	
HD2# 0.06100		CA 55.170000		RES_TYPE	PRO	CA 60.676000)
END_RES_DEF	,,,	HA 4.315000 CB 38.090000		SPIN_SYSTEM_ID	91	HA 4.204000	
mp_keg_ber		CB 38.090000 HB1 2.985000		HETEROGENEITY	100	CB 32.588000	
RES ID	793	HB2 2.661000		CA 63.980000		HB1 2.091000	
RES TYPE	GLN	END_RES_DEF		HA 2.422000 HB1 1.949000		CG 25.979000	
SPIN_SYSTEM ID	79	PWP_WPQ_PPF		HG1 1.648000		HG1 1.819000	
HETEROGENEITY	100	RES ID	799	HG2 1.558000		HG2 1.582000 CD 29.834000	
N 114.141000		RES_TYPE	CYS	CD 50.762000		HD1 1.813000	
HN 8.069000		SPIN SYSTEM ID	85	HD2 3.601000		CE 41.963000	
CA 59.024000	•	HETEROGENEITY	100	HD1 3.706000		HE1 2.962000	
HA 3.804000		N 116.928000		END_RES_DEF		END_RES_DEF	
CB 28.733000		HN 6.893000					
HB1 2.157000		CA 62.157000		RES_ID	806	RES ID	812
HB2 2.097000		HA 4.405000		RES_TYPE	GLU	RES_TYPE	CYS
CG 35.342000		CB 26.530000		SPIN_SYSTEM_ID	92	SPIN SYSTEM ID	98
HG1 2.460000		HB1 3.304000		HETEROGENE ITY	100	HETEROGENE ITY	100
NE2 111.3530		HB2 3.032000		N 112.993000		N 116.764000	
HE21 7.31900		END_RES_DEF		HN 8.246000		HN 8.520000	
HE22 7.22200	o .			CA 56.820000		CA 65.087000	
end_res_def		RES_ID	800	HA 4.185000		HA 4.202000	
RES_ID	794	RES_TYPE	LYS	CB 28.733000		CB 27.080000	
RESTYPE	ARG	SPIN_SYSTEM_ID HETEROGENEITY	86	HB1 2.095000		HB1 3.396000	
SPIN SYSTEM ID	80		100	HB2 1.973000		HB2 3.056000	
HETEROGENEITY	100	N 116.764000 HN 7.799000		CG 36.270000 HG1 2.200000		END_RES_DEF	
N 118.568000		CA 58.473000				BPC ID	012
HN 7.382000		HA 4.204000		END_RES_DEF		RES_ID	813
CA 58.473000		CB 32.588000		RES_ID	807	RES_TYPE	ALA 99
HA 4.078000		HB1 1.743000		RES TYPE	SER	SPIN_SYSTEM_ID HETEROGENEITY	100
CB 29.835000		CG 25.429000			93	N 120.700000	100
HB1 1.973000		HG1 1.313000			100	HN 8.315000	
HB2 1.886000		HG2 0.138000		N 115.780000		CA 55.563000	
CG 27.080000		CD 29.835000		HN 8.112000		HA 3.834000	
HG1 1.742000		HD1 1.291000		CA 58.473000		CB 18.270000	
CD 43.603000		CE 41.400000		HA 4.406000		HB# 1.597000	
HD1 3.390000		HE1 2.486000		CB 66.183000		END_RES_DEF	
HD2 3.325000		HE2 2.421000		HB1 4.393000			
end_res_def		END_RES_DEF		HB2 4.157000		RES_ID	814
				END_RES_DEF		RES_TYPE	ASN
			801				100
RES_ID	795	RES_ID				SPIN_SYSTEM_ID	100
RES_TYPE	VAL	RES_TYPE	GLU		808		100
		RES_TYPE			BOB GLU		

HN 8.068000 CA 56.27000 HA 4.329000 CB 38.64600 HB1 2.87700 HB2 2.83400 EMD_ERS_DEF RES_ID RES_TYPE	o o	RES_ID RES_TYPE SPIN_SYSTEM_ID HETERGEMEITY N 120.700000 HN 9.126000 CA 50.691000 HA 3.961000 CB 38.640000 HB1 3.289000	820 PHE 106 100	HB1 1.879000 HB2 1.757000 CG 24.878000 HG1 1.390000 HG2 1.302000 CD 29.284000 HD1 1.633000 CE 41.400000 HE1 2.913000 END RES DEF		END_RES_DEF RES_ID RES_TYPE SPIN_SYSTEM_ID HETEROGRWBITY N 125.450000 HN 7.774000 CA 57.720000 HA 4.082000	832 LYS 118 100
SPIN SYSTEM ID HETEROGENEITY N 119.880000 HN 7.912000 CA 65.08000 HA 3.646000 CB 39.19700 HB 1.924000 CGI 29.28400	o o	RES_TYPE	821 PHE	RES_ID RES_TYPE SPIN_SYSTEM_ID HETEROGENEITY N 121.192000 HN 8.063000 CA 59.024000 HA 3.995000	826 GLU 112 100	CB 33.410000 END_RES_DEF	
HGI1 1.88200 HGI2 1.20100 CG2 17.71800 HG2# 1.01700 * CD1 13.86300 HD1# 0.94000 END_RES_DEP	816	HETEROGENEITY N 118.076000 HN 8.359000 CA 61.770000 HA 1.840000 CB 38.090000 HB1 3.064000 CD1 133.24800	0	CB 29.834000 HB1 2.058000 CG 36.050000 HG1 2.342000 HG2 2.205000 END_RES_DEP RES_ID RES_TYPE	827 ALA		
RES_TYPE SPIN_SYSTEM_ID HETEROGENBITY N 122.504000 HN 8.556000 CA 56.820000 HA 3.670000 CB 41.951000 HB1 1.405000	LEU 102 100	RES_TYPE S	922 SER	- -	113		
HB2 1.199000 CG 26.530000 HG 1.580000 CD1 24.32700 HD1# 0.70100 CD2 25.429000 HD2# 0.696000 END_RES_DEF	0		108	RES_TYPE SPIN_SYSTEM_ID HETEROGENEITY N 126.767000 HN 7.744000 CA 45.902000 HA1 4.019000	828 GLY 114 100		
RES_TYPE SPIN_SYSTEM_ID HETEROGENEITY N 120.700000 HN 8.073000 CA 60.125000 HA 3.185000 CB 29.835000 HB1 1.720000 HB2 1.310000	817 GLU 103 100	RES_TYPE L SPIN_SYSTEM_ID 1 HETEROGENEITY 1 N 120.864000 HN 7.938000 CA 56.820000 HA 4.008000 CB 31.487000 HB 1.730000	123 .YS .09	RES_TYPE :	829 LEU 115 100		مئ <i>ن</i>
RES_TYPE SPIN SYSTEM ID	818 LYS 104	HB2 1.567000 CG 23.226000 HG1 0.833000 CD 27.080000 HD1 1.403000 CE 42.501000 HE1 2.569000 HE2 2.422000		CB 43.052000 HB1 1.562000 CG 27.632000 HG 1.536000 CD1 23.776000 HD1# 0.711000 END_RES_DEF	·		
HETEROGENETY N 117.584000 HN 7.145000 CA 59.688000 HA 4.075000 CB 32.588000 HB1 1.929000 CG 25.644000 HG1 1.492000 CD 29.284000 HD1 1.681000 CE 41.963000 HE1 2.964000 END_RES_DEF		RES_TYPE II SPIN_SYSTEM_ID 1:	24 LE 10 00	RES_TYPE I	130 LLE 1.16 0.00		
RES_TYPE SPIN_SYSTEM_ID :	100	CG2 18.820000 HG2# 0.654000 CD1 13.312000 HD1# 0.541000 END_RES_DEF		CD1 13.312000 HD1# 0.794000 END_RES_DEF RES_ID 8 RES_TYPE A	31 SP 17		
HA 4.328000 CB 39.200000 HB1 3.133000 HB2 3.047000 CD1 133.800000 HD1 7.180000 END_RES_DEF	1 5 2	ESS_TYPE 10 11 11 11 11 11 11 11 11 11 11 11 11	rs 11		00	•	

Unambiguous NOE-derived Inter-proton Distance Restraints

														•					
;	7.624	7.624	7.960	3.532		3.143		5.544	1.689	006.	5.053	2.613	2.698	2.790	3.208	4.40	9.113	4.811	4.010
	8.416 ppm2	8.924 ppm2	8.562 ppm2	. 872 ppm2		11.082 ppm2		8.001 ppm2	6.001 ppm2 6.001 ppm2			7.821 ppm2	7.823 ppm2	7.821 ppm2	8.936 ppm2	6.936 ppm2	0.936 ppm2	9.125 ppm2	9.125 ppm2
367668.00		0.43992E+03 ppm1	0.10017E+03 ppm1	0 72183E+02 ppm1		0.21046E+02 ppm1		0.52965E+03 ppm1	0.93421E+03 ppm1 0.18953E+04 ppm1		0.307908+03 ppm1	0.47343E+03 ppm1	0.16643E+03 ppm1	0.13090&+03 ppm1	0.90687&+03 ppm1	0.42952E+03 ppm1	0.45502E-03 ppm.1	0.72592E+03 ppm1	0.15487E+03 ppm1
0.11000E-01 volume	0.11000E+01 volume	0.11000E+01 voluma	0.11000E+01 volume	0.11000E+01 volume		0.11000E-01 volume		volume	0.11000K+01 volume 0.11000K+01 volume 0.11000K+01 volume	0.11080E+01 volume	0.11000E+01 volume	0.11500E+61 volume (0.11000E+01 volume (0.11000E+01 volume (0.11000K+01 volume (0.11000E+01 volume 0	0.110408+01 volume C	0.11000E+01 volume 0	0.11000E+01 volume (
name HN)) name HDt } 2141 weight g	HD22)) KE' } weight	HD211) HEN) weight	name HN)) name HDA) 8521 weight 0	NN)) NB1))		HO2 1)	neme HGI))	HN))	11 weight 0 name HW)) 21 weight 0		name HN)) name HA)) 41 weight 0	name HN }) name HB2 }} 51 weight 0	name NN)) name HG1)) 61 weight 0	name HN)) name HB1 j) 71 weight 0.	name HN 1) name HB4) 91 weight 0.	name HN)) name HA)) 101 weight 0.	name HN)) name HN)) 121 weight 0.	name HN)) name HA)) 131 weight 0.	neme HN)) neme HB1)) 141 weight O.
a a a		resid 89 and name resid 95 and name 1.500 peak 13271	resid 46 and resid 47 and 2.000 peak	resid 83 and name resid 88 and name 1.800 pask 14401	pu i		rasid 43 and resid 43 and	* * * * * * * * * * * * * * * * * * *	1.400 peak resid 41 and r resid 42 and r 1.200 peak	resid 42 and r resid 41 and r 2.200 peak	42 and 42 and 00 peak	resid 42 and n resid 42 and n 1.800 peak	resid 42 and n resid 42 and n 2.300 peak	resid 42 and n resid 42 and n 2.100 peak	resid 99 and n resid 99 and n 1.400 peak	resid 99 and n resid 99 and n 2.000 peak	resid 99 and n resid 98 and n 1.800 peak	reaid 98 and n reaid 98 and n 1.600 peak	resid 98 and n resid 98 and n 2.200 peak
and re	3.5	segid "BrD" and rea segid "BrD" and rea 4.000 4.000	megid 'BrD ' and rea aegid 'BrD ' and rea 3.500 3.100			### ##################################	segid BrD and ras [1] aegid BrD and ras (segid BrD and res	2.700 1.800 (11) segid 'BrD " and rea	4.400 4.21) 96914 BrD and res 96914 BrD and res 2.200	eegid BrD and reseegid BrD and res	aegid "BrD " and reaid aegid "BrD " and reaid 2.900 2.100 2.1	rD and res	10 * and 10 * and 2.600	rD and res		rD " and res		and res	ord " and res 2.700
2141) **91d 4.200	ASSI (13261) ((segid ") (segid ") 3.900	((segid ") (segid ") (segid ")	((segid ") (segid ") 3.500 ASSI (14401)	((eegid " ((eegid ").700 OR (14401)		([aegid **	ASSI (aegid ") ((aegid ") ((aegid ")	2,700 ASSI (11) ((asgid "E (asgid "E	ASSI (21) ((869id °E ((869id °E (2.200	ABSI (31) ((segid "B ((segid "B 3.300	Abs: (aegid B (aegid B 2.900	((segid 'B ((segid 'B 2.700 ASSI (61)			((megid "B (megid "B 2.400 ASSI (101)	((aegid "B ((aegid "B 2.800 AEEI (121)	((megid 'B ((megid 'B 2.700		((segid "g (segid "g 1,300

3.696	5. 45				oct : 6			.00	2.307	1.409	3.596	4.59	9.164	4.977	4.201	3.95		. 84	3.740	6.476	. 56	3.43
9.125 ppm2	12.275 ppm2	12,275 00002			7	131 e		6. 479 ppm2	8.480 ppm2	8.166 ppm2	8.166 ppm2	6.165 ppm2	6.166 ppm2	7.738 ppm2	7.740 ppm2	7.729 ppm2	12.275 ppm2	5.488 ppm2	6.487 ppm2	9.740 ppm2	9.740 ppm2	P. 740 ppm2
0.95273E-03 ppm1	0.20628£+03 ppm1	0.16806E+03.ppm1	0.404638.03				0.12405K.03 ppm1	0.13933E+03 ppm1	0.88455E+03 ppm3	0.829526+03 ppm1	0.71632K-03 ppm1	0.53058E+03 ppm1	0.11688E+03 ppm1	0.656215+03 ppm1	0.308726+03 ppm1	0.59972E+03 ppmt	0.41861E+03 ppm1	0.22043E+03 ppm1	0.42542E+01 ppm1	0.44987E+03 ppm1	0.55394R+03 ppm1	0.71868E+03 ppm1
0.11000E+01 volume	0.11000\$+81 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000£+01 volume	200000	0.31000E.01	0.11000£+01 volume	0.110008+01 volume	4.00.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 Volume	0.11000£+01 volume	0.11050£+01 volume	0.11000£.01 volume	0.11000E+01 volume	0.11000E+01 volume	0.110008+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000S+01 volume	0.11000E+01 volume
151 weight	name KN)) name NA)) 171 weight	name KW)) name KB1)) 181 weight	name HN)) name HB2)) 191 weight		name HW))	name HN 1) name HB1 1) 221 weight		name HM)) name HA)) 241 weight	name KN 1) name HB1) 251 velght	name HN 3) name HB2 3) 271 weight	name HM }} name HB1 }} 281 weight	name KN)) name KA)) 291 weight	name HM)) name HM)) 301 weight	name HN }) name HA)) 121 weight	name HN)) name HB1)) 331 veight	name HN 1) name HB2 1) 341 weight	name HN)) name HN)) 351 weight	name HN)) name HA)) 361 weight	name HW)) name HB1)) 371 weight	name HM)) name HM)) 401 weight	name HN)) name HA)) 411 weight	eme HBL }}
reald 98 and 1.400 peak	resid 30 and resid 30 and 2.400 peak	resid 30 and resid 30 and 2.300 peak	resid 30 and resid 30 and 2.000 peak	reeld 30 7-eld 29 2.200	reald 29 and reald 29 and 3.600 peak	* * * * *	reald 31 and reald 39 and 2.100 peak	resid 31 and resid 31 and 2.200 peak	resid 31 and resid 31 and 1.400 peak	resid 28 and resid 28 and 1.600 peak	resid 28 and resid 28 and 1	resid 28 and resid 28 and 1.800 peak	resid 28 and resid 29. and 2.100 peak	resid 32 and s resid 32 and s 1.700 peak	resid 32 and resid 32 and 2.100 peak	reald 32 and r reald 32 and r 1.700 peak	resid 30 and r resid 31 and r 2.000 peak	resid 105 and n resid 105 and n 2.400 peak	resid 105 and n resid 105 and n 2.000 peak	resid 106 and n resid 105 and n 1.800 peak	resid 106 and n resid 106 and n 1.700 peak	maid 106 and n 1.600 peak
.400 1.400	gad "BrD " and paid "BrD " and 100 2.400	sgid BrD and sgid BrD and 2,600	eagld BrD and 1 eagld BrD and 2.800	201) 1914 "BrD " and 1 1914 "BrD " and 1 100 2.700	211) 4gid "BrD " and egid "BrD " and .700 1.800	221) 1914 "BrD " and 1 1914 "BrD " and 1	(231) segid "BrD " and 1 aegid "BrD " and 3 3.400 2.900	aegid BrD and aegid BrD and 3,300	egid BrD and a egid BrD and a 2.400 1.400	eegid "BrD " and r aagid "BrD " and r 2.500 1.600 [281]	segid BrD and r 2.500 1.600	eegid BrD and r 2.700 1.800	aegid BrD and r 3.400 2.900	aegid BrD and r aegid BrD and r 2.600 A.700	eegid 'BrD' and r eegid 'BrD' and r 2.900 2.100 [341]	gid '8rD * and r gid '8rD * and r 600 1.700	aegid BrD and r aegid BrD and r 2.800 2.000	gid "BrD " and r gid "BrD " and r 100 2.400	d 'BrD * and d 'BrD * and 0 2.000	220	eegid "BrD " and ry aegid "BrD " and ry 2.600 1.700	megid 'BrD' and re aegid 'BrD' and re 2.500 1.600 (431)
7 188	=======================================		- # # A.	A881	A681 C C C C C C C C C C C C C C C C C C C	ABS1 C C C 2.2 2 2.2	A881		ASST 2.	((as	2.	(ee (e	, (se	((se		1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	A881	7 I	((eegic ((eegic 2.600	== }		

7.983

4.612 ppm2

0.57823E+03 ppm1

4.980

7.996 ppm2

volume

3.337

ī d

ASSI (741) ((aegid "BID " 4 (aegid "BID " 4 2:700 1:60 ABBI (791) ((aegid "BID " 4	ASSI (1713) (1840 - 1.46	ASSI (791) (1 megid "BrD" (1 megid "BrD"	2.600 1,70 ASSI (811) ((8egid "BrD " 4 ((8egid "BrD " 4	3.200 2.20 ASSI (641) ((6egid 'BrD "	2.600 1,70 ASSI (851) (aegid BRD - a		• ~ ~ •	((aegid BED = 2.500 1.70 ASE (aegid BED = 4.70 ((aegid BED = 4.70	((segid 'BrD ' 3.100 2.40 ABSI (901)	4 ~ ~ 3	2 700 2 700 (921)	megid 3.300	i i	• • ~ ~ •		(aegid BrD 2.500 1.60	1 6 4 4	((eegid arp = 2.500 1.60 A8SI (1041)	14-14		((eegid 'BrD " a 2.100 1.10 ASSI { 1091} ((eegid 'BrD " a	8 % 8
2 2	ř	*	ř	ž	7	¥	¥	¥	2	84	84	SK .	84	*	87	84	¥	PAS	AB	Y	ء مشر	-
3.674		1.43	3.671	1.966	4.011	4.583											9.	2.667	4.904	1.967	4.619	40.4
9.740 ppm2		4.941 ppm2	8.960 ppm2	8.529 ppm2	6.526 ppm2	8.526 ppm2	6.572 ppm2	6.714 ppm2	8.714 ppm2	8.714 spm2			6 16 a	8.714 pom2	667 2092	6.668 ppm2	8.668 ppm2	8.668 ppm2	6.217 ppm2	6.219 ppm2	8.376 ppm2	6.219 ppm2
0.11996E+04 ppm1	0.11255E+01 ppml	0.57631E+03 ppm1	0.16715E+03 ppm1	0.57313E+03 ppml	0.52916E+03 ppm1	0.97894E-03 ppm1	0.11922E+04 ppm1		0.43619E+03 ppm1									0.15417E+04 ppm1	0.42876E+03 ppm1	1mdg [0+3f1000.0	0.42782E+03 ppm1	0,73858.01 pml
0.11000E+61 volume	0.11000E+01 volume	0.11000K+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11500E+01 volume	0.11000E+01 volume	0.11000£+01 volume	0.11000K+01 volume	0.110006+01 volume	0.110008+01 volume								0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E.01 voluma
segid "9:0" and resid 106 and name HB2)) 3.00 11.300 11.300 peak 431 weight (451) and name HB)) 3.900 21.00 peak 431 weight (5.50) 21.00 peak 431 weight (5.50) 21.00 peak 431 weight	reald 107 and name resid 107 and name 2.000 peak 461	meid 107 and name meid 107 and name 1.700 peak 471 med name	resid 107 and hame 2.300 pmsk 481 resid 108 and name	1.700 peak 501	meald 10s and name HN)) reaid 10s and name HA)) 1.800 peak 511 weight	meid 108 and name HB1)) seid 108 and name HB1)) 1.400 peak 521 weight		[481] (eegid '81) and resid 110 and name HN !) (eegid '81D and resid 109 and name HR2 !) 2.900 2.100 2:100 peak 541 weight		eaid 110 and name HN)) eaid 110 and name HB)) 1.600 peak 561 weight	seid 109 and name HN)) seid 110 and name HN)) 2.000 peak 581 weight	maid 111 and name HN }} asid 108 and name HA }} 2.300 peak S91 weight	celd 111 and name HW)) seld 111 and name HA)) 1.600 peak 601 weight	esid 110 and name HN }} esid 111 and name HN }} 2.000 peak 621 weight	meid 112 and name HN)) seid 112 and name HA }) 1.300 peak 631 weight	mesid 112 and name HN)) esid 112 and name HG1)) 2.100 peak 641 weight	seid 112 and name HN)) seid 112 and name HG2)) 2.000 peak 651 weight	esid 112 and name HN)) esid 112 and name HB1)) 1.200 peak 661 weight	meid 113 and name HN)) meid 113 and name HA)) Z.DGO peak 671 weight	esid 113 and name RN !) ssid 113 and name RBt) 1.400 peak 681 waight	1 (70) and read 114 and name HN)) aegid "BED" and read 114 and name HA1)) 3.60 2.00 2.000 peak 701 weight 731 veight	eegid 'BrD' and resid 113 and name HH) eegid 'BrD' and resid 114 and name HH) 2.500 1.600 peak 721 weight
A561) 188 Y	7381 7381	Nes :	Ass.)	== }	==	1 = 1	==	is ex	A881	1884	Yesi	Assi C C C	7881 () ()	YSSE .	iger V			==	=======================================	==

3.422

1.669 ppm2

volume

ppm2

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VO. LINE

1,664

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. 936

volume

4.809

1.676 ppm2

6.672 ppm2

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1.977 ppm2

3.995

7.976 ppm2

0.420918+03 ppm1

volume

3.113

7.979 ppm2

6.678

7.979 ppm2

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0.11000E+01 volume

1.1

8.669 ppm2

1 1 2

3.596

.669 ppm2

volume

741 wight
741 wight
742 wight
743 wight
744 wight
745 wight
745 wight
745 wight
745 wight
746 wight
747 wight
748 wi

designation of the control of the co

1.11

.679 ppm2

0.13526E+03 ppm1

3.346

8.669 ppm2

6.670

9.679 ppm2

5.037

1.713 ppez

0.16612E+03 ppm1

volume

4.753

4.713 ppm2

6.873 ppm2

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volume

.871 ppm2

611 ppm2

6.612 ppm3

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volume

ASBI (1331) (megid 'BrD ' and resid	2.600 2.000 (1401)		ASSI (1411) ((segid "SrD " and resid ((segid "BrD " and resid	2.400 1.400 (1411)			3.200 2.600		segid 'BrD " and re segid 'BrD " and re 2.500 " And re	ASSI (1471) (1 megid 'Bro and read	2.600 1.700 (1481)	((segid "BID " and reald ((segid "BID " and reald 2.400 1.400 1.4	~ • • •	ASSI (1501)	(eegid BED end regid 2.100 1.100 1.30 ASEI { 1521}	(segid 'BrD ' and resid (segid 'BrD ' and resid 2.700 1.800 1.80		ASSI { 1541} ((eegid "BrD " and reald 2	(megid "BID " and resid 2 2.300 1.300 1.30 ABBI (1561)	(megid BrD and resid 2 ((megid BrD and resid 2 2.90 2.100 2.100	(seeid 'BrD ' and resid M(seejd 'BrD ' and resid M(seejd M(BrD ' and resid M(BrD ') and resid M(BrD	ASSI (1581) ((megid "BrD " and resid 20 ((megid "BrD " and resid 20	2.700 1.800 1.81 ASSI (1.851)	[(eegid "Brp" end resid 2) [(eegid 2) 2,700 2,200 A581 [1601]	({ eegid 'BrD " and reald 23 (eegid 'BrD " and reald 23 2.600 1.700 1.700 ASSI (1611)	((megid 'BrD " and resid 23	((segid 'BrD " and resid 23 ((segid 'BrD " and resid 23 2.100 2.100 2.100 A&ST (1641)	BrD and 1.700	(eegid 'BtD - and reaid 15 (eegid 'BtD - and reaid 15 ASSE (1641) 2.400 3.400 ASSE (1641) 2.400
4.527	5		3.221	2.919		2.616	80.6		7.004	4.368	3		2.903	7.535		-	4.357	4.690	2.923		1.549	1.410	6.022	;		5. 14.2	3.669	J. 52.6	# # # # # # # # # # # # # # # # # # #
9.104 ppm2	9.106 ppm2		9.106 ppm2	9.106 ppm2		9.106 ppm2	0.613 ppm2		7.536 ppm2	7.516 ppm2	7.535 post		7.836 ppm2	9.105 ppm2			6.019 ppm2	8.306 ppm2	8.306 ppm2		6.306 ppm2	8.306 ppm2	8.106 ppm2			Tadd or	Zudel	6.622 ppm2	
0.40919E+03 ppm1	0.66185R+03 ppm1		0.30957E+03 ppm1	0.19539E+03 ppm1		0.72202E+03 ppm1	0.517928+03 ppm1	:	U.14234K+03 ppm3	0.2311E+03 ppm1	0.42552E+03 ppm1		0.473868+03 ppm1	0.42446B+03 ppm1	0.785592-01 prest			.43607E+03 ppm1	0.13733E+03 ppm1	:		0.243358+03 ppm1	0.40402E+03 ppm1	0.347368403 press			0.525518-01-001	3	0.2007sE+03 ppm1
0.11000E+01 volume	0.11000E+01 volume		C. IIOOUE+OI VOLUMA	0.11000E+01 volume		• 401 M	0.11000E+01 volume			0.11000E+01 volume	0.11000E:01 volume		e m	0.11000E+01 volume	0.11000E+01 volume (0.110008.01		0.11000E+01 volume 0.	0.11000K+01 volume 0	0.110008401		.11000£+01 volume 0	0.11000E.01 volume 0	0.11000E+01 volume 0		100	volume	volume	0.11000E+01 Volume G.
1111	and name MG1)) peak 1121 weight	and name HN)) and name HO2))	and has	11	and name HN)) and name HB2)) peak 1151 maicht	1	end name KN)) Seak 1171 weight	and name HN 1) and name HDt) peak 1181 weight	name HN))	1191 weight	And name HB1)) Peak 1201 weight	and name HN)) and name HB2))	name HN))	1231 weight	and name RN)) and name RA')) Peak 1241 weight o	and name KN)) and name MB2)) peak 1251 weight o	22	1261 weight	HB))	and name HN)) and name HG10) peak 1261 weight 0	name HN))	name HN ()	1301 weight	and name HN)) and name HDA) peak 1321 weight 0.	and name HN)) and name HA }) Peak 1331 weight 0.		•	HN)) HN)) weight o	and hame HN)) and name HD%) peak 1381 weight 0.
2.000 2.000	1.700	and resid 75 and resid 75 2.100 2.100	and resid 75	2.400	##914 BrD and resid 75 ##914 BrD and resid 75 2.500 1.600 1.600 p	at bies	1.	2.200	27 bis	2.200 2.200	2.000	egid BrD end resid 74 egid GrD end resid 74 1.700 1.800 p.	24 Dist	2.000	1.600	2.100	63 bie	2.00d	2.200	aid 63 2.000 P	14 69 14 69	9	2.00	11d 68 2.100	2.300	1d 68	2 5 6 5 1 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	14 69 14 69 2.000	2.400
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3.549 1.429 5.001 3.627 1.342 2.659 8.765 4.527 1.135 4.669 2.534 4.367 2.486 4.645 3.143 2.939 7.663 4.132 ppm2 6.812 ppm2 6.833 ppm2 1.622 ppm2 0. 626 ppm2 4.564 ppm2 8.565 ppm2 4.763 ppm2 1.566 ppm2 8.544 ppm2 6.565 ppm2 4.546 ppm. 6.146 ppm2 0.147 ppm2 6.146 ppm2 6.514 ppez 9.456 ppm2 9.123 ppm2 9.114 ppm2 9.119 ppez 9.118 ppm2 4.598 ppm2 ((segid "BrD " and resid 24 and

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	0.61276E+03 ppm1	0.32851E+03 ppm1	0.39507E+03 ppm1	0.374758+03 ppm1	0.17051E+01 ppm1	0.42952E+03 ppm1	0.19765E+03 ppm1	0.11203E+03 ppm1	0.62404E+03 ppm1	0.28244E+01 ppm1	0.28579E+03 ppm1	0.44735R+03 ppm1	0.15320E+03 ppm1	0.22276E+03 ppm1	0.72297£+01 ppm1	0.26347E+03 ppm1	0.26996E+03 ppm1	0.10141E+04 ppm1	0.62488R+03 ppm1	0.36079E+03 ppm1	0.49246E+03 ppm1	0.02312E+03 ppm1	0.726058+03 ppm1
	0.110005+01 Volume	0.11000E.01 VOLUME	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000£+01 volume	0.11000£+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000K+01 volume	0.11000\$+01 volume	0.11000£+01 volume	0.11000E+01 volume	0.11000E-01 volume	0.11000\$+01 volume	0.11000E+01 volume	0.11000E-01 volume	0.110008+81 Volume	0.11000E+01 volume	0.11000K+01 volume	0.11000E+01 Valume
	a a a	and name and name peak 1981	and name	1	and name and name peak 2021	and name and name Peak 2011	and name and name peak 2051	and hame and name peak 2061	and name and name peak 2071	and name and name yeak 2081	and name and mane wak 2091	aid 87 and name HN 1) aid 87 and name HB2 }} 1.800 peak 2101 weight	and hame HN)) and hame HD%) peak 2111 weight	and name and name peak 2121	and name HN }} and name HB1 }} peak 2131 weight	and name HM 1) and name HA 1) peak 2151 weight	and name HB1)) peak 2161 weight	Δ.	end name HN)) end name HN)) peak 2191 weight	and name NN)) and name NN)) peak 2201 weight	and name HN)) and name HA)) peak 2211 weight	and name KN)) and name HB1)) peak 2221 weight	and name HB2)) and name HB2)) peak 2231 weight and name HW))
11.61	aegid "BrD " and resid 83 aegid "BrD " and resid 84 2.600 1.700 1.700 [1981]	eegid BrD end resid 65 eegid BrD end resid 65 2.900 2.100 2.100	megid "BrD" and resid as megid "BrD" and resid as 2.000 2.000 2.000 [2011]	megid "BtD" and resid 84 megid "BtD" and resid 85 2.800 2.000 2.000 { 2021}	megid "BrD" and resid a6 megid "BrD" and resid 85 1.200 2.600 2.300 2031}	megid BrD and resid so megid BrD and resid so 2.800 2.000 2.000	agid BrD and resid es	megid BrD and resid of aegid BrD and resid of 3.400 2.900 2.100 (2011)	aegid BrD and resid 87 8-81d BrD and resid 87 2.600 1.700 1.700	14 BrD and resid 67 and 14 BrD and resid 67 and 00 3.200 2.200 peak 091)	megid "BrD" and resid 87 megid "BrD" and resid 67 3.000 2.200 2.200 [; ;	"BrD " and reald 88 "BrD " and reald 88 2.700 2.200	2.400		2.300	2.200	1.400	1. 700	2.000	meid 46 meid 46 1.800	resid 46 resid 46 1.600	segid 'BrD' and resid 46 segid 'BrD' and resid 46 2.500 1.600 1.600 [2241] segid 'BrD' and resid 47
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661	6 6 0 ppg	8 . 654 Dom2				9.112 ppg2	9.133 ppm2	9.133 pom2	8.661 ppm2	9.196 ppm2	6.169 ppm2		Zudd over e	2mgq 2.1.0			9.169 ppm2	5.446 ppm2		Fudd Accord		7.444 ppm2	9.463 ppm2
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and name HA)) peak 1661 weight	and name and name peak 1671	and name and name pesk 1681	and name and name peak 1691	and name HN)) and name HN)) peak 1711 weight	and name HN)) and name HA)) peak 1721 weight	and name HM)) and name HB)) peak 1731 weight	and name HN)) and name HGIt) peak 1741 weight	and name HN)) and name HG2V) peak 1751 weight	and name HW)) and name HW)) Peak 1771 weight	and name HW)) and name HA)) peak 1791 weight	and name HN }) and hame HB1 }) peak 1801 weight		name HN)) name HB1)) 1821 weight	name HN)) name HN))	and name HN }} and name HA }} peek 1851 weight	and name NN)) and name NA))	and name HN)) and name HN))	and name HM)) and name HA)) sek 1901 weight	name HN)) name HB))				
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| 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.800 | 2.80

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{ 2521} eegid "BrD" and resid 51 and n aegid "BrD" and resid 51 and n 2.900 2.100 2.100 pask 2	0.40 2.20	(2541) Aegid BED and reaid 17 and n Regid BED and reaid 17 and n 2.400 1.400 1.400 pask 2	[253] Begid "BrD" and resid 17 and n segid "BrD" and resid 17 and n 1,100 2,400 peak 2		serial BrD and resid 101 and pegid BrD and resid 101 and resident 2 and	4914 "BtD * and resid 100 and regid "BtD * and resid 101 and refer 100 peak 7	(segid "BrD" and resid 102 and r (segid "BrD" and resid 102 and r 2.100 pask 2	411) 91d "BFD" and resid 102 and n 91d "BFD" and resid 101 and n 700 1.800 1.800 peek 2	BrD " and resid 103 and n BrD * and resid 103 and n 2.000 2.000 peak 2	1851, 1954 BFD and resid 103 and regid BFD and resid 103 and regid BFD and resid 103 and resid 105	BrD * and resid 103 and n BrD * and resid 103 and n 1.600 1.600 peak 2	91d "BrD" and resid 103 and n gid "BrD" and resid 103 and n 200 2.600 2.900 peak 2	2681) egid "BrD" and resid 101 and c egid "BrD" and resid 102 and r 600 1.700 m 1.700 peak 3	711) id BID and resid 104 and id BID and resid 104 and of 00 1.700 peak	2731) gid "BrD" and reald 104 and name M gid "BrD" and resid 101 and name M 800 2.000 2.000 pask 2731 w	2751} gid "BrD" and resid 104 and r gid "BrD" and resid 105 and n 700 1.800 pask 2	3.80 a.m.	2781} egid "BTD" and resid 81 and name H egid "BTD" and resid 81 and name H .300 2.700 2.300 peak 2781	(2791) eegid "BrD" and resid at and n eegid "BrD" and resid at and n 2.500 1.600 pask 2	1.600	1 2213 1 eggid "BrD" and resid 81 and n eggid "BrD" and resid 81 and n 3.100 2.400 2.400 peak 2	2.200 p	*BrD * and resid #2
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7.253	4.70	3.807	3.391	4.815	2.83	2.63	6.310	0.69	2.611	1.506	7.743	9.310	4.525	8.554	4.542	4. 822	2.169	4.828	2.419	\$.171	3.300	3.147	4.475
6.632 ppm2	8.831 ppm2	6.633 ppm2	6.832 ppm2	8.307 ppm2	8.104 ppm2	8.108 ppm2	6.632 ppm2	7.762 ppm2	7.762 ppm2	7.762 ppm2	8.308 ppm2	8.559 ppm2	6.544 ppm2	7.762 ppm2	8.355 ppm2	8.355 ppm2	8.086 ppm2	8.067 ppm2	8.086 ppm2	8.880 ppm2	6.879 ppm2	8.879 ppm2	4.377 ppm2
0.71965E+02 ppm1	0.34426E+03 ppm1	0.370838+03 ppm1			0.14081E+03 ppm3	0.110188+04 ppm1	0.47004E+01 ppm1	ė	0.22961E+03 ppm1	0.15115E+03 ppm1		0.55001R+03 ppm1	0.45800E+01 ppm1	0.91502E+03 ppm1	0.20145E+03 ppm1	0.36367E+03 ppm1	0.51528E+03 ppm1	0.81456E+03 ppm1	0.560858+03 ppm1	0.15334E-03 ppmi	0.14660K+03 ppm1	0.41931E+03 ppm1	0.136438+04 ppm1
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0.900@46+02 ppm1	0.34424E+03 ppm1	0.30448E-03 ppm1			. \$5403E.03 ppm1	0.220116+03 ppm1	0.21874E+03 ppm1	3	57256E+03 ppm1	0.19260&+03 ppm1	0.81267E-03 ppm1	0.88513E+02 ppm1	0.23859E+03 ppm1	0.66455E+03 ppm1	0.747716+03 ppm1	0.67721E+03 ppm1	0.16876E+03 ppm1	0.157158+03 ppm1	0.131068*04 ppm1	.151728+03 ppm1	39310E+03 ppm1	8E.02 ppm1	
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0.187248+03 ppm1 0.23212E+03 ppm1 0.57314E+03 ppm1	0.93460E+02 ppml 0.17148E+03 ppml 0.1143SE+03 ppml	0.18238E.03 ppm1 0.91130E.03 ppm1 0.11008E.03 ppm1	0.14843E.03 ppm1 0.87461E.03 ppm1		0.11966E+03 ppm1 0.65813E+02 ppm1 0.88464E+02 ppm1	0.11541E+03 ppm1 0.88336E+02 ppm1 0.86531E+02 ppm1	0.13498c01 ppm1 0.10932c01 ppm1 0.47519c01 ppm1
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10 Mare 10 1	U.11000K+01 volume	e 0.11556E+04 ppm1	7.974 ppm2	5.542	690))	egid BrD and reaid 66 and name	and name KN))	•		
ishe HB1)	0.11000E+01 volume	0.71474E+02 ppm1	7.975 ppm2	2.572	2.7 ASSI { 4	000 1.800 1.800 per	ak 4801 weight	0.11000E+01 volume	0.46166E+03 ppm1	9.76
Labor HN))	0.11000E+01 volume	B 0.20373E+03 pom3	7.878		4-6 4-6 5-8)	2, 100	and name NN)) and name NB1)) peak 4811 waight	0.11000E+01 volume	0.11537E+03 ppm1	.78
AMERIN)) AMERIKA)) SSI weight		0.363646.0			ee) 1854	asid 66 asid 65 2.200	and name HB2)) and name HB2)) peak 4821 weight	0.11000£+01 volume	0.11653E+03 ppm1	6.763
ame KN)) ame KB1)) \$61 weight			rundd		((eng (eng (eng 2.0	2.000	and name HW)) and name KA)) peak 4833 weight	0.11000E-01 volume	0.418\$\$E+03 ppm1	
Ame KN)) Ame KA)) 571 weight			port of the state		(resid 68 resid 67 2.100	and name HA)) and name HA)) peak 4841 weight	0.11000E+01 volume	0.12732£+03 ppm1	1.637
Ame KN)) Ame KA)) 581 weight	0.11000£+01 volume		10.050 mm		((eeg) ((eeg))).3(2.200	and name NN 1) and name NB2 1) peak 4851 weight	0.1100dE+01 volume	0.152138+03 ppm1	.626
Ame HM))	0.11000E-61 Volume				((mg/) (1.400	and hame HW)) and name HA)) peak 4861 weight	0.11000E+01 volume	0.95815E+03 ppm1	. 305
Ame HN)) and HB)) 601 weight	0.11000E+01 volume				(1 669. 7. 50 4. 50 8. 1	5 pind 6	115	0.11000K+01 volume	0.22391E+02 ppm1	• 304
Ame HW))	0.11000E+01 volume		48 Carre		((eeg) ((eeg) 3.30 ASSI (48	amyid 'BrD ' and resid 69 and 1.300 2.700 2.200 peak		0.11000E+01 volume	0.15981E-03 ppm1	.306
and HN 1)	0.11000E+01 volume	0.1703415-03	10.051 pom2		(aegi (aegi 3.00 8.51 (49	Z.	I name HN)) I name KA)) 4891 weight	0.11000E+01 volume	0.24418+03 ppm1	•.03
ine HN))	0.11000E+01 volume	0.89496	243		(eegi (eegi 1.49 3.40 Agg { 49	2.100 pa	hame HB)) 4901 weight	0.11000K+01 volume	0.12954E+03 ppm1	0.040
ine RN)) ine HB2)) ist weight	0.11000E+01 volume	0.72876E-03 pmm1				X.	name HH:)) name HGIV) 4911 weight	0.110008+01 volume	0.61869E+02 ppml	.041
ine HN)) ine HA)) is) veight	0.11000E+01 volume		748 0000			d BED and resid 70 and d BED and resid 69 and 100 1.800 peak	name HM)) name HG24) 1921 weight	0.11000E+01 volume	0.48346E+03 ppm1	0.040
me HN)) me HN)) 91 veight	0.11000E+01 volume	0.96369E+03 ppm1	8.566 ppm2	35	15er))	X.	name HA))	0.11000K+01 volume	0.30696E+03 ppm1	. 045
me KN)) me KA)) 01 weight	0.11600E+61 volume	0.17192R+03 ppm1	4.997 ppm2	959.4		wested "BED" and resid 74 and mested "BED" and resid 71 and 1.500 2.000 peak [4951]	NAME NO 1)	0.11090E-01 volume	0.10430E+03 ppm1	7.536
ne HN)) In Hoight	0.11600E+01 volume	0.35764E+03 pgm1	9.477 ppm2	6.6	(2.000 :	Name KN))	0.11000K+01 volume (0.10099E+03 ppm1	9.106
me HN)) me HA)) 31 weight	0.11006E+01 volume	0.90728E+02 ppm1	9.472 ppm2	1481	(# # # # # # # # # # # # # # # # # # #	2.100	name HW)) name HA)) 4961 weight	0.11000E+01 volume 6	0.11734E+03 ppm1	1.611
me KD21)) me HB1)) 41 weight	0.11000g+01 volume	0.10454E+03 ppm1	8.206 ppm2	1.61		2.200	name HO1))	0.11000E+01 volume 0	0.26326E+03 ppm1	.611
me HD22)) me HB1)) 51 weight	0.11000E+01 volume	0.97769E+02 ppm1	7.576 ppm2	3.637	108A 108.6 1	egid "BrD" and reald 75 and 1.200 2.400 peak	name HG2))	0.11000E+01 volume 0	0.18815E+01 ppm1	6 . 6 10
me HD21)) me HB2)) 61 weight	0.11000E+01 volume	0.17534E+03 ppm1	6.205 ppm2	3.393	2. (See)	1 "BrD and resid 76 and 1 "BrD and resid 75 and 1.700 1.700 peak 11.	name HB2))	0.11000E+01 volume 0	.e19648+03 ppm1	1.611
Me HD22))	.11000E+01 volume	0.13182E+03 ppm1	7.576 ppm2	3.393) (A691 2.600 A691 (SO)	aegid BrD and read 7s and 2.600 1.700 peak [5 501]	SOOL Weight	0.110008-01 volume 0	.59739E+03 ppm1	1.611
ne KE21)) ne HG1)) 11 veight (0.11000ft+01 volume	0.11561E+03 ppm1	7.634 ppm2	3.459	1 (2 () () () () () () () () ()	2.200 P	name HA)) 5011 waight	0.11000K+01 volume 0	0.25554E+03 ppm1	7.386
me HE22)) me HG1)) bl weight (0.11000E+01 volume	0.90206E+02 ppm1	7.523 ppm2	3.474	1884	segid "BTD" and resid 75 and 45011}	Soll weight	0.11000E+01 volume 0	0.86259E+03 ppm1	7.94

| 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,000 | 1,00

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8.014 ppm2

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1.13

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0.105156+03

6.553

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4.115

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7.586

8.458 ppm2

0.19134E.03 ppm1

4.559

6.856 ppm2

0.89575£+01 ppm1

4.400

6.858 ppm2

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2.77

6.658 ppm2

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0.16189E+02 ppm1

3.059

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0.38088E.02

2.997

0.486 ppm2

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1.314

6.480 ppm2

0.14151E+03 ppm1

d resid 31 and name H fresid 102 and name H 2,200 peak 11311 w

2.742

7.73 ppm2

0.57286E+02 ppm3

d resid 32 and name H 1.600 pesk 1331 w d resid 32 and name H d resid 33 and name H d resid 33 and name H 1.600 pesk 13341 w

2.174

7.739 ppm2

0.82617E+03 ppm1

4.975

1.183 ppm2

0.11000E.01

and name and name peak 11381

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2.784

8.181 ppe2

0.60528E+03 ppm3

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resid 34 and name P 1.700 peak 11411 v Festd 34 and name P 2.200 peak 11421 v

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resid 34 2.200 p

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8.184 ppm2

1.094

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Volume

and name and name peak 11461 and name and name Pug

resid 34 2.000 p

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1.364

8.680 ppm2

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9.003 ppm2

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	and name and ness sak 12331	and name and name	and name	esk 12351	and name	and name and name ask 12371
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0.103	0.	0.857		9.11		9.611	0.333	0.31672	6.433	0.66		0.156						0.70	9.12	9.33	71.0	0.181008	9.3
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0.173986-02 ppm1	0.26713E+03 ppm1	0.81254E.01 ppm1	0.18836E+02 ppm1	0.40043£+02 ppm1	0.121688+02 ppm1	0.383388+02 ppm1	0.49230E+02 ppm1	0.9997E-di ppml	0.12922E+02 ppm1	0.54819E+03 ppm1	0.951496+01 ppm1	0.232538-02 ppm1	0.212678+02 ppm1	0.22190E-02 pm1	0.119178+02 ppm1	0.18067E+02 ppml	0.254378+02 ppm1	0.283808+02 ppm1	0.32802E+01 ppm1	0.25780E+02 ppm1	0.42831E+01 ppm1	
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	0.22594E+02 ppm1		0.549698+02 ppml	0.81305K+03 ppm1	0.43435E+02 ppm1	0.161648+02 ppm1	0.15931E+02 ppm1	0.45701£+03 ppm1	0.31541E+02 ppm1	0.21235£+02 ppm1	0.901598+02 ppm1	0.40125E+02 ppm1		0.18909E+02 ppm1	0.631428+03 ppen	0.13744E+02 ppm1	0.16187E+03 ppm1	0.533025+02 ppm1	0.21172#+02 ppm1	0.30250K+02 ppm1	0.71559E+02 ppm1	0.14584K+02 ppm1	
on to avoid the		0.10000E+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000£.01 volume	0.19000E+01 volume	0.10000E+61 volume	0.10000E+01 volume (0.100008+01 volume (0.10000\$+01 volume (0.10000E+01 volume (0.10000E+61 volume (0.10000K+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.100008+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000K+01 volume 0	
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19 and name HM })		12 and name NG1))	and name	ă.	and neme	and name HB1)) peak 15081 weight	and name HN !)	Peek 1	and name	and name KO1))		and name KN))		8 and name KE1 ())	(NH same pur)	O peak 15161 weight (0 and name HM))	ask 15171 weight	and name HN)) and name HN))	All seed box	and name HB1 1) Peak 15201 weight	and name KM)) and name HD10) mak 15211 ceroby		resid 26 and name HS1)) 1.100 peak 15261 weight o	and name	Δ.	and name KN)) and name HE22)) peak 15311 weight	and name HW)) and name ME21))	and seed been	and name HR) and name HR) peak 15161 weight	and name HW)) and name HG)) peak 15391 weight	and name KN 1) and name KN 3) peak 15401 weight	and name HN))	peak 15421 weight	and name HN)) and name HN)) peak 15441 weight o	and name HN)) and name HD16) peak 15481 weight		and name NA)) peak 15511 weight o
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0.475488+03 ppm1	0.208108+03 pps1	0.21305E+03 ppm1	0.21514E+03 pgm1	0.22249E+03 ppm1	0.23254E+03 ppm1	0.45818E+03 pom	0.31584E+03 ppm1	0.94493K+02 ppml	0.184716+03 ppm1	0.28741E+03 ppm1	0.23932E+03 ppm1	0.28555E+03 ppm1	0.17185E+03 ppm1	0.168988+03 ppm1	0.36354K+03 ppm1	0.761235.03 ppm1	0.87848E+03 ppm1	0.10742E+04 ppm1	0.84264E-03 ppm1	0.277016+03 ppm1	0.16922E+03 ppm1	0.10996E+01 ppm1	
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name HD24) 1462 weight 0.11	name HB1 1) name HA 1) 8552 weight 0.11	name MB2)) name HD1%) 8562 weight 0.11	name HA)) name HB)) 8602 weight 0.11	name HD11) name HA)} 8652 weight 0.11	name HD34) name HD31) 8672 weight 0.11	name HD24) name HD14) 8662 weight 0.13	name HA)} name HBA) 8722 weight 0.11	name MD14) name MB1)) 8742 weight 0.11	name KA) name KE¢ 6752 wasght 0.11	name HB1)) name HB4) 8782 weight 0.11(name MB2 1) name MEN) 8792 weight 0.11	neme HB1)) neme HA))			KDIA)	HD21) HG21)		name HD24) name HE4) 8912 weight 0.110	name HA 1) neme HB1)) 8922 weight 0.110	ime NA)] ime NB2)) i32 veight 0.110	hamme HB1)) namme HA)) 8952 weight 0.110	name KD1V) name KA. 1) 6972 weight 0.110	me MD14) me MB1)) e2 weight 0.110
reald 102 and r	seld 33 and seld 19 and 1.700 peak	eeid 22 and eeid 22 and 1.600 peak	resid 22 and resid 25 and 1.700 peek	resid 56 and resid 56 and 1.600 peak	resid \$6 and resid 78 and 2.100 peak	resid 56 and resid 78 and 1.300 peak	seid 73 and seid 76 and 1.400 peak	meid 73 and meid 73 and 1.400 peek	esid 76 and esid 59 and 2.200 peak	resid 78 and resid 59 and 2.300 peak	resid 78 and resid 59 and 2.100 peak	reeld 78 and reeld 75 and 2.400 mask	resid 78 . and	resid 76 and resid 81 and	resid 78 and 2.100 peak	resid 78 and resid 25 and 1.700 peak	resid 78 and resid 81 and 2.000 peak	resid 7s and resid 59 and 1.700 peak	resid 102 and resid 105 and 2.000 peak	resid 102 and na resid 105 and na 1.800 peak 89	111	¥ 8 8	reeld 102 and na reeld 108 and no 3.200 peek 63
aegid BrD and 5.500 5.500	megid 'BrD * and megid 'BrD * and 2.600 1.700	aegid 'BrD ' and i aegid 'BrD ' and i aegid 'BrD ' and i 2.500 1.600	megid BrD end 1 megid BrD end 1 2.600 1.700	eegid BrD and eegid BrD and 2.500 1.600	segid BrD and 2.300 2.100	segid 'BrD * and segid 'BrD * end 2.300 1.300	segid BrD and segid BrD and 2.700 1.800	segid 'BrD ' and a segid 'BrD ' and a 2.400 1.400	eegid "BrD and eegid "BrD and 3.300 2.700	eegid BrD and eegid BrD and 1.200 2.600	segid BrD and 2.900 2.900	(8802) aegid "BrD " and aegid "BrD " and 3.100 2,400	(8812) 8891d 'BrD * and 8891d 'BrD * and 3.200 2.400	[8822] eegid "BrD " and eegid "BrD " and 2,600 1,700	megid 'BrD " and megid 'BrD " and 2.900 2.100	270 • 070 2.700	id 'BrD and 1d 'BrD and 1d 'BrD and 00 2.000	id BrD and id BrD and 00 1,700	egid "BrD " and egid "BrD " and 1,800 2.000	d BrD and d BrD and o 1.800	segid 'BrD * and 1 2.900 2.100 [8972]	egid 'BrD and :egid 'BrD and :.700 1.800	egid "BrD " and
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1.271	ppm2
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1.807	2) yper 5
4.810	ppm2
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2.857	ppm2 3.
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4.775	bpers

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3.340 ppm2

4.296

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4.289

2.781 ppm2

2.585 ppm2

1.236

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3.781

4.304 ppm2

1.55

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4.359 ppm2

4.756 ppm2

5.143

2.634 ppm2

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2.501 ppm2

2.784

\$.051 ppm2

5.046

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36

0.52255£+03 ppm1	0.74419E-02 ppm1	0.30562E+03 ppm1	0.14886K+03 ppm1	0.14114E+03 ppm1	0.34604E+03 ppm1	0.13575E+03 ppm1	0.116765-03 ppm1	10.331.035		0.53477E+03 ppm1	0.59437E+03 ppm1	0.11894E+01 ppm1	0.15710£+03 ppm1		0.117766:03 ppm1	0.48585K+02 ppm1	0.47917E+02 ppm1	0.15116E+03 ppm1		tedd foregentst o	0.12572E+03 ppm1	0.94017E-02 ppm1	0.132616+02 pps1	0.10292K+03 ppm1	0.56479E+02 ppm1	0.82899K+02 ppm1
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and name MG1 1) pak 10752 weight and page MA 11	and name 10763	and name HB1)) tak 10792 weight	and name HB1))	and name HA 1) and name HB2 1) peak 10812 weight	aid 27 and name HB1)) aid 24 and name HA)) 1.600 peak 10822 weight	and name HB1)) and name HB1)) eak 10932 weight	and name MA)) and name MB2)} mak 10942 weight	and name HA 1) and name HD1 1) tak 10952 weight	and name KG2)) and name KD1))	and name MD1))	poak 11012 weight	and name HA)) and name HB1)) peak 11092 weight	and name HD1)) and name HB2)) peak 11112 weight	and name HD1))	and ness (U)	peak 11152 weight	and name HDZ)) and name HDZ)) pask 11162 weight	and name HD1 1) and name HD1 1) peak 11212 weight	and name NG2)) and name ND1))	and name (402))	peak 11232 weight	and hamm MD2 3) peak 11242 weight	and name MO21) peak 11252 weight	and name	and name MB1)) and name MD14) pask 11292 weight	and name MB2 } and name MD1%} peak 11302 weight
*BrD * and resid so 1.300 1.300 }	2.600 2.300	((segid 'BrD " and resid 9 2.500 pt 1.600 pt 1.	*BrD * and reald 23 2.000 2.000	2.100 2.100		9.9	= =		99	or of or	1.30	2.200 2.200	2.000	aegid "BrD " and reaid 11 aegid "BrD " and reaid 10 3.200 2.200	9	2.100	2.100	2.000	(111414) second MrD and reald 53 second @rD and reald 53 2.800 2.800	23	2.100	(megid 'BrD " and reald 53 3.100 2.400 2.400 [[11252]	1. 200 1. 200	2.200	2.200	segid "BrD" and resid 19 segid "BrD" and resid 63 3.400 2.900 2.100
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		•																							J.	
2.780	4.873		;	7.07	1.145	2.729	2.731	1.731	4.738	4.634	4.507		2.931	2.647	2.662	2,662		2.181	966.1	1.703	3.60	4.951				4.672
4.854 ppm2	2.779 ppm2	2.585 ppm2		rudd cac r	3.782 ppm2	4.803 ppm2	4.831 ppm2	2.570 ppm2	2.694 ppm2	2.684 ppm2	2.684 ppm2		4. 509 ppm2	4.509 ppm2	3.523 ppm2	3.227 ppm2		\$. 000 ppm2	2.141 ppm2	5.000 ppm2	\$.000 ppm3	2.536 pom2	: 3	y and d	4.536 ppm2	2.584 ppm2
.30668E+03 ppm1	0.28367E+03 ppm1	0.80939K+03 ppm1			0.42729E+02 ppm1	0.46141E-03 ppm1	0.564028+03 ppm1	0.48724E+03 ppm1	0.12901E+04 ppm1	0.44320E+03 ppm1	0.38447E+03 ppm1		0.361448.03 ppm1	0.19358K+03 ppm1	0.23961R+03 ppm1	0.23485E+03 ppm1		0.25166R+03 ppm1	0.30460E+03 ppm1	0.46749E+03 ppm1	0.87656E+03 ppm1	0.24800E+03 ppm1				0.13820K+03 ppm1
0.11000E+01 volume 0	0.11000E*01 volume 0	0.11000K+01 volume 0	0 110000010		volume.		0.11000E+01 voluma 0	.110005+01 volume 0	0.11000E.01 volume 0	0.11000E+01 volume 0	0.11000E-01 volume 0		0.1IUDOK+Ol volume 0	0.11000E+01 volume 0	0.11000E+01 volume 0	0.11000E+01 volume 0		0.11000E+01 volume 0	0.11500E+01 volume 0	0.11000K+01 volume 0.	0.11000E+01 volume 0	0.11000E+01 volume 0.				0.11000E.01 volume 0
4))	161 161 191 191 191 191 191 191 191 191		and name HB2 () and name HB1 ()	HG2))	# 13ht	weight HA))	weight HB2))	peak 10452 weight 0 and name HB1))	Me 1ght	4 1 1	1	: :	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	weight HOI))	and name HEV) tak 10552 weight	and name HG2)) and name HE's) sak 10562 weight	and name KA)) and name KG1))	and name HG2))	and name KA))	KB1)	and name MA 1) and name HB2 1) peak 10662 weight 0.	and name HB2)) and name HA)) peak 10672 weight 0.	HB1))		1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Waaght I
(10322) eegid 'BrD' and resid 67 and name 1 eegid 'BrD' and resid 87 and name 1 2.500 1.600 pack 10322 v	and resid 67 and resid 64 1.700 1.700 pe	1.100	resid 87	seid 87	2. dbo	1.400	1.300 eeid 92	1.300	1.000 1.000 pr	" and resid 109 and name 1.400 1.400 peak 10482	* and resid 112 and name H * and resid 112 and name H 1.400 1.400 peak 10492 w	and resid 75	osid 7	1.400 20 14	1.700 1.700 pe	(segid "BrD " and reald 75 segid "BrD " and reald 75 2 600 1.700 pc	and resid 66	1. 700 1. 700 1. 700 1. 700	1. 600 1. 600	1.300	1.100	eeld e0	00 bis 00 77 1.700	on pie	of bies	2.100
ASSI [10322] ({ megid "BID ({ megid "BID (megid "BID	(1 eegid "BrD" and r (1 eegid "BrD" and r 2.600 1.700	ASSI (10342) ((esgid "BrD - and r ((esgid "BrD - and r 2.100 1.100	ABSI (10352) ((megid "BTD " and ((megid "BTD " and 2,300 1,300	(10392) eegid 'B'	1.500 3.100 ASSI (10402) ((segid "BrD * and r ((segid "BrD * and r	2.400 1.400 ABSI (10423) ((segid "BrD * and i ((segid "BrD * and i	2.300 3 AGSI (10452) ((segid "BrD	2.300 1.300 ASSI (10462) ((megid 'BrD " and r	2.000 ASSI (10482) ((eegid "BrD	(f eegid "BrD end 2.400 1.400 ABSI (10492)	((megid "BrD " and r ((megid "BrD " and r 2.400 1.400	A681 (10512) ((eegid 'BrD ' end r ((segid 'BrD ' end r	ASSI [10542] ((megid 'BrD " and x (megid 'BrD " and x	2.400 ASSI (10552) ((eegid "BrD	1 8eg1d BrD and r 2.600 1.700 ASSI (10562)	(segid BrD (segid BrD 2.600	ASSI (10632) ((megid 'BrD ((megid 'BrD	ASSI [10642] ((megid "BrD ((megid "BrD	2.500 1.600 ASSI [10652] ((eegid "BrD " and re	((segid "BrD 2.300 ASSI (10662)	([eegid BiD end r (eegid BiD end r 2.100 1.100	((segid 'BiD ' and i ((segid 'BiD ' and i 2.600 1.700	A5SI {10662} ({ segid "BrD " and r ({ segid "BrD " and r 2.600 1.700	ASSI (10692) ((segid "BrD " and 1 ((segid "BrD " and 1	A581 [10702] ((eegid "BrD " and re ((eegid "BrD " and re	2.900 2. Asst {10753} {{ segid 'SID *

4.7

4.608 ppm2 4.801 ppm2 4.403 ppm2

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2.857

4.901 ppm2

2.931

4.901 ppm2

2.33

4.655 ppm2

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2.337

4.803 ppe2

4.337

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4.312 ppm2

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3.300

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3.35

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5.446

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4.015 ppm

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4.011

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2.290 ppm2 2.290 ppm2

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0.13883E+03 ppm1	0.12386E+63 ppm1	0.11534E+03 ppm1	0.97663E+02 ppm1	0.132438+03 ppm1	0.13995E+03 ppm1	0.343468.03		ration to the control of	0.16299E+02 ppm1	0.52760E+03 ppm1	0.19334E+03 ppm1		0.59031E+02 ppm1	0.905786+02 ppml	0.13057£+03 ppm1	0 300745.03		0.108268+03 ppm1	0.42931E+03 ppm1	0.81117E+01 ppm1			.42022K+03 ppm1	.403198-02 ppm1	0.38368E+03 ppm1	0.51224E+03 ppm1	
0.11000E+01 volume 0	0.11000\$+01 volume 0	0.11000E+01 volume 0	0.11000E+01 volume 0	0.11000E+01 volume 0	0.11000E+01 volume 0	0.11000E+01 volume 0	-		0.11000E+01 volume 0	0.11000E+01 volume 0	0.11000E.01 volume 0		U.IIGGGE-GI VOLUME D	0.110005+01 volume 0	0.11000E+01 volume p	0.11000E+01 volume 0		0.110008+01 volume 0	0.11000E+01 volume 0	0.11000K+01 volume 0	o Thompson to a		0.110605.01 volume 0.	0.110008+01 volume 0).11000E+01 volume 0.	0.11000£+01 volume 0.	_
and name HB2)) peak 12032 weight	and name NG2 } and name NB2 } peak 12042 weight	and name and name peak 12062	and name and name pask 12072	and name HD1)) and name HO2)) peak 12062 weight	and name HD2)) and name HG2)) peak 12092 weight	and name KB1)} and name KG2)} pmak 12103 weight	and name HB1)) suid name Hill))	and name (KA))	20121 32 P	and name HG2)) and name HEV) peak 12222 weight	and name HEt) and name HEt) peak 12342 weight	and name MA))	and name NA 1)	end name HBI }) peak 12262 weight	and name NA)) and name NB2)) peak 12272 weight	and name HB1)) and name HA)) peak 12312 weight	and name NB1))	peak 12322 weight	and name (A.)) peak 12332 weight	and name HB2)) and name HA)) peak 12342 weight	and name HD24) and name HG))	and name HD21)	and name HD24)	and name MB1) peak 12422 weight	and name peak 12432	and name MD10) and name HB2)) peak 12442 weight	and name HD1%) and name HB1 }) peak 12452 weight
BrD * and 2.100	eegid BrD = and resid 13 eegid BrD = and resid 13 2.900 2.100 2.100 [12062]	segid 'BrD ' and resid 33 segid 'BrD ' and resid 33 3.000 2.200 2.200 [12072]	megia "BrD" and resid 33 megid "BrD" and resid 33 1.100 2.400 2.400 12082}	segid "BrD" and resid 13 segid "BrD" and resid 13 2.900 2.100 2.100	segid "BrD " and resid 33 segid "BrD " and resid 33 2.900 2.100 2.100	megid "BrD" and resid 33 eegid "BiD" and resid 33 2.900 2.100	(12132) segid "BrD" and resid 33 segid "BrD" and resid 33		22) 4.100 1.400	megia "arp and reald 59 eegid "BrD " and reald 59 2.300 1.300 1.300 (12042)	segid "BrD" and resid 59 angle "BrD" and resid 59 2.700 1.800 1.800	megid "BrD" and resid 59 [megid "BrD" and resid 59] 1000 2 200 2 200		aegid BrD and resid 62 3.100 2.400 2.400 [12272]	2,100	eegid "BrD " and reald 61 eegid "BrD " and reald 61 2.500 1.600 1.600	BrD . and	2.200	1.400 1.400	rD * and re rD * and re 1.100	22	pue . Qu	1.400 PrD * and Fe	1 *BrO * end resid 31 3 3.100 2.000 pc 32}	segid Brb and resid 14 2.400 1.400 1.400	segid "BrD" and reald 14 segid "BrD" and reald 14 2.300 1.300 1.300	(12452) 4 4444 "BrD" and resid 14 5 4444 "BrD" and resid 14 2.300 1.300 1.300
((eegid ", 2.900 2.900 AS&I (12042)	((eegs. (eegs. 2.90 ASSI (120	ASSI (130	((eegid 3.100 ASB1 (12002		(eagl (eagl (eagl (eagl	(eeg.	ASSI (121) ((aegic ((aegic		4.10 ASSI (122	(segid 's 2.300 ASSI (12342)	(eegic eegic 2.700	300 ())))))))))))))))))	ASSI [12262] ((aegid "B	{ segid *B 3.100 ASSI (12272)	(eegid '8 2,900 ASSI (12312)		ASSI (12322) ((eegid "B ((eegid "B	3.000 ASSI (123)	(megid *B 2.400 ASSI (12342)	((segic () segic 2.100	Abbi (1458) (segid (segid 2.000	ASSI (12402) (aegid "B (aegid "B	ASSI (12422) (segid "E	(segid " 3.500 ASSI (12632)	([aegid "E 2.400 ASSI [12442]	2.300	ASEI (1245 (megid (megid 2.300
•				4.807	0.766	4.667	4.667	16	1,646	ļ.		0	4.911		·	978		5.643		•	651	651	•	611	;	į	<u>a</u>
A BOS.				7.340 ppm2 4.6	2.340 ppm2 0.7	2.636 ppm2 4.6	2,190 ppm2 4.6	4.972 ppm2 2.291	2.291 DOM2 4.6	ļ	3.177 ppm2 2.323	2.629 ppm2 1.480	3.177 ppm2 4.9		Ĺ	5.347 ppm2 2.978	5.347 ppm2 2.708	6.559 ppm2 5.6		4.410 ppm2 3.66m	2.710 ppm2 4.559	2.978 ppm2 4.559	2.725 ppm2 5.378	4.361 ppm2 -0.319	9		4.360 ppm2 1.083
0.408718+03 press				o.sate7keds ppms	0.122618.03 ppm1	0.48201E+03 ppm1	0.27261K+03 ppm1	.40526K+03 ppm1	0.26243B+03 ppm3		0.19040K+03 ppm1	0.69523E+02 ppm1	0.81736E+02 ppm1	0.119638+01		0.18441E+03 ppm1	0.32384E+02 ppm1	0.19122E+03 ppm1		0.16567E+03 ppm1	0.31825E+02 ppm1	0.50256E+02 ppm1	0.17033E+03 ppm1	0.10731E+03 ppm1	0 200608.03 prest		0.18669E+03 ppm.1
0.11000£+01 Volume 0.	, and a	01 volume	<u> </u>		0.11000K+01 volume 0.	0.11000E-01 volume 0.	0.11000E+01 volume 0.	.11000E.01 volume 0.	.11000E+01 volume 0.		. 11000K+01 VOLUME 0.	0.11000E+01, volume 0.	0.11000E+01 volume 0.	0.110008+01 volume 0.		0.11000K+01 volume 0.	0.11000£+01 volume 0.	.11000E-01 volume		d.iloddkedl Volume G.	0.110008+01 volume 0.	0.11000£+01 volume 0.	.11000£.01 volume 0.	.11000E+01 volume 0.	0.11000K+01 volume 0		.11000E+01 volume 0.
and name HA)) and name HG1)) ask 11392 weight	and name HB1)) and name HA)) tak 11422 weight	and name HD1)) and name HA)) mak 11442 weight	and name HB1)) and name HA))	and name HB1))	eak 11462 weight and name HB1)) and name HA))	ank 11612 weight and name HG1))	and name KA 1)	and name ask 11692	and name HD1 and name HA peak 11702 weight 0	and name	and name	and name HD1))	and name HA)) tak 11742 weight	and name HG1)) and name HD2)) peak 11782 weight 0		H ight	a 1ght	end name NOI)) and name NA)) eak 11852 weight 0	and name HD2))	and name HB2)	nk 11912 weight	ok 11922 weight	•	and name HA)) and name HG2)) peak 11952 weight 0.	and name HA)) and name HB2)) peak 11962 weight 0.	49	weight o
### (11392) ####################################	II (11422) (segid "BrD " and reald 97 (segid "BrD " and reald 94 2.200 1.200 1.200 p	(11442) eegid "BrD " and resid 97 eegid "BrD " and resid 97 3.600 3.200 1.900 p	<pre>if (11472) [(eegid "BrD " and resid 86 [(eegid "BrD " and resid 86 2,400 1,400 p. 1,400 p.</pre>	rD * and resid 86	4.300 2.100 2.100 p [[11612] [Aegid BrD * and Feaid 64 [Aegid BrD * and reald 61	1.300 1.300 gr ro and resid 64 rd resid 64	2.600 1.700 1.700 p. (11692)	1.400 1.400 p	rD and resid 72 1.700 1.700 p	rD and resid 62	rD and resid 62	2.300	2.400 2.400	aid 91 2.200	16 2	1. 800 1.	7	1.000 1.000 p	i tites; [segid 'BrD ' and resid 9] [segid 'BrD ' and resid 9]	rD * and reeld 91	1.600	2.900 2.100 pr	2.000	2.200	1. 800 1. 800	CC bies	.800 1.800
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3.7 8 1 p	4.409 p	4. 409 p	2.680 p	4.630	4.901	2.560 p	2,145 p	1.303 p	1.305 p	1.303 g	0.911 g	. 44.		. 904	4.163 ppm2	1.164	3.078 g	2.372	3.570 F	2.63	4.705	1,376 ppm2	
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and name and name peak 14012	aid 79 and name aid 82 and name 2.200 peak 14072	and name and name peak 14082	said 79 and name said 76 and name 1.400 peak 14092 v	sid 94 and name sid 97 and name 2.300 peak 14182	seid 113 and name leid 17 and name 1.900 peak 14252	3 3 4	resid 14 and name resid 11 and name 2.200 peak 14572	seld 102 and name beid 31 and name 2.100 peak 14592 v	resid 102 and name resid 25 and name 1.300 peak 14612	sid 102 and name sid 25 and name 1.800 peak 14622	and name and name peak 14662	\$ \$ ¥	3 3 4	3 3 3	8 8 4	\$ 8 ¥	888	8 8 4	3 3 3	3 3 4			
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•		aegid "BrD - and resid 74 and name HB1)] aegid "BrD - and resid 74 and name HD1) 2.900 2.100 2.100 peak 13412 weight	degid BED and resid 74 and name NB2)) segid BED and resid 74 and name NE%) 3.00 2.300 1.900 pusk 15482 weight (1549)	degid BED and resid 74 and name HB1)) eegid BED and resid 74 and name HEV) 2.000 2.000 2.000 peek 15492 weight	segid 'BED' and rasid 82 and name HB2 segid 'BED' and rasid 82 and name HE\$ segid 'BED' and rasid 82 and name HE\$ 1.000	115914 BID end resid 82 and name segid BID and resid 82 and name 2.800 2.000 peak 15612	[137] [137	12742 12742	(1934 BT) and resid 15 and name HA 1) eegid "BTO" and resid 18 and name HD34) 4.600 4.600 0.900 peak 15792 weight	(Regid 'BrD' and resid 107 and name HA)) eegid 'BrD' and resid 107 and name HE) 7.700 1.800 1.800 pesk 16522 weight	degid BED and rasid 56 and name MA)) segid BED end resid 56 and name HEt) 2.000 2.000 2.000 pask 16532 weight	[6691d 'BFD and resid 52 and name HA]) (6691d 'BFD and resid 53 and name HG2)) 5.500 5.500 0.000 peak 16692 waight	1909id 200 200 200 200 200 2.0		(eegid BED and resid 105 and name HB2)) eegid BED and resid 105 and name HD1) 2.00 1.300 1.300 pask 17202 weight		(1-6914 PED - and resid life and name HA) (eegid 'BrD - and resid life and name HG12) 2-800 2.000 peak 17292 weight (13103)	(segid "BrD " and resid 116 and name HA11) (segid "BrD " and resid 116 and name HA11) 3.100 2.400 paak 17102 weight (1742)	(eegid 'BrD * and resid 34 and name MB2)) segid 'BrD * and resid 34 and name MD4) 3.500 2.100 2.100 peak 17412 weight		2.600		segid '91D * and resid 33 and name ND2) segid '91D * and resid 33 and name NB2) 3.000 2.200 2.200 peak 17812 weight
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0.283025+03 ppm1	0.13602E+03 pps	0.55156E+01 ppm1	0.52712E+02 ppm1	0.28846E+03 ppm1	0.19930K+01 ppm1	0.38344£+03 ppm3	0.91919K-02 ppm1	0.66608E+02 ppm1	0.22677E+02 ppm1	0.75265E+02 ppm1		0.3\$265£+02 ppm1	0.29199£+03 ppm1	0.271228+03 ppm1	0.38647£+03 ppm1	0.162138+03 ppm1	0.58337E-01 ppm1	6.311538+03 ppm1	0.36307E+03 ppm1	0.11465E-05 pps1	0.511118.02 ppm1	0.15234E+03 ppm1).94082E+02 ppm1
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2.63	3.177	3.177	2.62	2.5	2.641	1.69	2.641	1.501	2.340	4.459	1.747	1.751	1.747	1.056	1.056	1.056	0.740	1.155	1.155	2.634	2.634	2.634	
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1.090	0.925	3.525	3.835	. 508	4.507	•	4.370	4.370	3.074	4.753									3.30	2.598	4.847	4.947	1.788
1.498 ppm2	1.494 ppm2	1.989 ppm2	2.290 ppm2	1.694 ppm2		3.124 ppm	3.469 ppm2	3.076 ppm2	6.744 ppm	3.917 ppm2	1.797 pgm2					1.153 ppm2	35		1. 09.1 DOM2	1. and paper	2.519 ppm2	3.598 ppm2	3.129 ppm2
0.19359E+03 ppm1	0.2041E-01 ppm1	0.20066£•02 ppm1	0.655\$78+02 ppm1	0.12761E+03 ppm1	0.50116E+03 ppm1	0.91712K+02 ppm1	0.67606E+02 ppm1	0.26410E+03 ppm1	0.62910E+03 ppm1	0.879298+02 ppm1	0.55437E+03 pcm1				0.117156.01	0.314148.03 ppm;	0.970\$2\$+02 mm1		0.14101E+04 ppm1	0.62174E-03 ppm1	0.45243E+02 ppm3	0.23440E+02 ppm1	0.14855K+03 ppm1
0.11d0qE+01 volume	6.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E-01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	.11000£+01 volume	0.11000E-01 volume	0.11000E-01 volume			0.11999E-91 volume	0.11000E+01 volume	.11000E+01 volume	0.11000£+01 volume	0.11006E-01 volume	0.11000g.01 volume	9.11000E+01 volume	.11000E+01 volume
16 and name HD1%) 800 peak 24662 weight	and name MD24) and name MB2 1) peak 24672 weight	resid 19 and name MB2) resid 19 and name HE1) 1.500 peak 24742 weight	and name HB1)) and name HB1)) peak 24752 weight	and name HOl)) and name HA)) peak 24762 wasght	and name HD1 }) and name HA 1} pest 24812 weight	and name MO1)) and name MA)) peek 24872 weight	and name HG1 }) and name HA }) peak 24902 weight	resid 24 and name MG2) resid 21 and name MA) 1.700 peak 24912 weight (reeld 24 and name HA)) reeld 24 and name HB1)) 1.200 peak 24912 weight	and name HB1)) and name HA)) ik 25432 weight	101 and name HG12)) 101 and name HB) 100 peak 2552 weight (21 and name MG24) 18 and name MA)) 200 peek 25612 waight (resid 110 and name HD14) resid 75 and name HG1)) 2.100 peak 26032 weight (HO20) HD20)	MD11) HD21)	Light 1	resid 103 and name MA }} resid 106 and name MDN } 2.400 pesk 26562 weight 0	nd name KB1)) nd name KA)) k 26592 weight	and name KB2)) and name KG2)) mak 26642 weight	resid 103 and name HB2)) resid 103 and name HO1 }) 1.200 peak 26652 weight 0	reeid 103 and name HG2 }) reeid 100 and name HA 1) 2.000 pask 26662 weight 0	and name HG1)} and name HA }) esk 26672 weight (94 and name MG1)) 32 and name MH2)) 100 peak 26722 weight 0
segid "BrD " and resid 2.700 1.800 1.6		segid BrD and resid segid BrD and resid 4.000 4.000 1.8			segid "BrD " and resid 19 segid "BrD " and resid 16 12 100 1.300 1.300 1.300 1.300 1.300 1.300 1.300	megid "BrD" and resid 23 megid "BrD" and resid 20 3.100 2.400 2.400	eegid "BrD " and resid 24 megid "BrD " and resid 21 3.200 2.600 2.300 [24812]	eegid "BrD " and resid segid "BrD " and resid 2.600 1.700 1.7	segid 'BrD ' and resid segid 'BrD ' and resid 2.200 1.200 1.2	megid "BrD" and reald \$5 seegid "BrD" and reald \$2 see 3.100 3.400 3.400 pee	megid "BrD" and resid 101 cegld 201 cegld 200 1.300 pe	eagid "BrD" and resid 21 amgid "BrD" and resid 18 amgid "BrD" and resid 18 amgid 18	[36032] segid BrD • and resid segid BrD • and resid 3.400 2.800 2.1	{24172} megid "BrD " and resid megid "BrD " and resid 4.400 4.400 1.1	(24182) eegid "BrD " and resid eegid "BrD " and resid 3.000 2.200 2.3	(26102) segid "BrD and segid "BrD and 1.500 1.600	26562} egid 'BrD ' and egid 'BrD ' and 1,100 2,400	(26592) segid BrD and resid 103 a segid BrD and resid 100 a 2.700 1.800 1.800 pea	[26642] emgid "BrD " and resid 10] 7,000 1.000 1.000 p	amegid "BrD" and resid amegid "BrD" and resid 2.200 1.200 1.20	eegid BrD and resid megid BrD and resid 3.500 3.300 2.00	: :	eegid BrD and resid eegid BrD and resid 2.900 2.100 2.1
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	7,998	7.785	1.731	1.900	7.031		.5.	4.376	3.955	3.890	5.542	5.366	4.306	1.362	3.286	2.463	7.259	7.259	4.110	5.540	4.110	3.134	4.383
	2.735 ppm2	2.733 ppm2	3.123 ppm2	3.762 ppm2	2.779 DDM2				2.536 ppm2	2.536 ppm2	2.336 ppm2	2.979 ppm2	1.058 ppm2	1. 699 ppm2	1.899 ppm2	1.600 ppm2	0.760 ppm2	0.662 ppm2	1.549 ppm2	1.253 ppm2	1.253 ppm2	1.254 ppm2	1.303 ppm2
	8+03 ppm3	Beal ppm1	E-03 ppm1	8+02 ppm1	E+03 ppm1		ē	ş			E+00 ppm1	8+03 ppm1				ē	8		E+03 ppm1	8-02 ppm1			R+03 ppm1
	luma 0.359368+03	volume 0.100898+01	volume 0.72439E	volume 0.348748+02	volume 0.47090≝+03		volume 0.27730g.	Volume 0.16302E	volume 0.12614E+03	Volume 0.14981E+03	Volume 0.478418+00	volume 0.722718	volume 0.91001E+02	volume 0.14735E+04	volume 0.70123E+03	volume 0.12667E	Volume 0.39776E	Volume 0.49710g+03	voluma 0.10505E+	Volume 0.259308+03	Volume 0.48455E+02	volume 0.68625E+02	Volume 0.89519E+03
	0.11000E-01 volume	0.11000E+01 vo	0.11000E+01 vo	0.11000E+01 vo	0.11086E.01 vo		0.11000E+41 VO	0.11000E+01 vo	0.11000E+01 vo	0.11000E+61 vo	0.11000E+01 vo	0.11000E+01 Vo	0.11000K+01 vo	0.11000E+01 vo	0.11000£+01 vo	0.11000E+01 vo	0.11000E+01 Vo	0.110008+01 vo	0.11000E+01 vo	0.11000E+01 VO	0.11000E+01 vo	0.11000E+01 vo	0.11000E+01 vo
He HB1))	MB1 13	weight (()	e ight	KD1))	HB1)) HG1))	HD2))	HDI))	HB1)	HB2 1) HD1 1)	KB2)) HD2)) weight	HO 1)	KB1 1) KA 1)	HOIV) HBI))	KD2V) KG)) veight	KB2 () KB2 ()	HD24) HB2)) weight	HD16) HD1)	KD2V) KDV) veight	HB1))	HD24) HA 1)	HB1))	ND24) NB2 1)	HD14)
94 87 87 87 87 87	500 peak 26782 94 and name	36 pack 267	1.200 peak 26842	86 and name 100 pask 26862	id 87 and name id 87 and name 1.400 peak 26882	80 and name 80 and name 100 peak 27152	80 and name 80 and name 100 peak 27162	1	\$ \$ *	2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	4 4 4	SS and name 55 and name 00 peak 27352	81 and name 34 and name 00 peak 27412	2 5 4 2 5 4	\$ 5 5 5 \$ 5 5 5	73 and name 73 and name 00 peek 27682	2 to 2	78 and name 62 and name 00 pask 27972	56 and name 34 and name 00 peak 28242	56 and name 34 and name 00 peak 28282	56 and name 34 and name 00 peak 28312	56 and name 34 and name 100 peak 28362	eid 102 and name aid 102 and name 1.100 peek 28672 eid 102 and name
(26782) aegid "BrD" and resid 94 Becald "BrD" and resid 12	.600 1.600 end resid 94	200 2.200 and resid 94	200	and resid \$6.200	11	and resid so and resid so	and resid so and resid so	2 and resid 77 2 and resid 74 2.000 2.000	and resid so and resid so	and resid 80 and resid 80	and resid 56 and resid 34 .500 0.000	end resid 55 and resid 55	and resid 81 and resid 34	D * end resid 22 D * end resid 22 0.900 0.900	0 * and reald 22 0 * and reald 22 1.200 1.200	0 * and resid 73 D * and resid 73 2.100 2.100	2 2	and resid 78 and resid 82 .900 2.100	and resid S6 and resid 34 .200 2.200	D • and resid 56 D • and resid 34 3.600 1.700	and resid 56 end resid 34 .900 2.100	2.600 2.300	
		3.000 2.200 [(26842) [eegid 'BrD ' and r	2.200 1 (26862)	3.500 3.200		[27152] eegid 'BrD ' and a eegid 'BrD ' and 2.400		[37212] segid 'BrD ' and segid 'BrD ' and 2.800 2.000	segid BrD and 32.900 3.100	eegid BrD and eegid BrD and 2.500	megid BrD and segid BrD and 5.500 5,500	segid 'BrD and r	aegid BrD and r eegid BrD and r 3.100 2.400	27512) segid BrD end segid BrD end 1.900 0.900	- 6 6 4-	eegid Br	segid BrD and segid BrD and J. 600	eegid BrD and 3.400 3.900	1887	aegid 'Br	7 8 8 7 2	eegid 'BrD and eegid 'BrD and 3,200 2,600 (28673)	megid 'Bri 2.100 (28712)
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0.12274&.04 ppm1 0.4012X+03 ppm1 0.44400E+03 ppm1 0.12446E+03 ppm1 0.12446E+03 ppm1 0.12446E+03 ppm1 0.1242E+03 ppm1 0.1242E+03 ppm1 0.26228E+03 ppm1 0.26228E+03 ppm1 0.26228E+03 ppm1	0.2014E+02 ppm1 0.20544E+03 ppm1 0.20544E+03 ppm1 0.211345E+03 ppm1 0.17274E+03 ppm1 0.17274E+03 ppm1 0.17274E+03 ppm1 0.17274E+03 ppm1 0.17274E+03 ppm1 0.17274E+03 ppm1
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(10112) 9egid "BrD" and resid 66 and name HBl)) 9egid "BrD" and resid 96 and name HR) 2.700 1.300 1.	(10192) segid 'BrD' and resid so segid 'BrD' and resid so	30402) 10402)	2.200 1.200 3.200 1.200 [30412]	segid 'BrD and 2.900 2.100	segid 'BrD' and segid 'BrD' and 2.900 2.100	eegid 'BrD and regid 'BrD and r	2.400	segid BrD and segid BrD and 2.700 1.800	# 512 P	eegid BrD and r eegid BrD and r 1.700 0.700	segid BrD and segid BrD and 2.500 1.600	10872) megid WrD and r megid WrD and r 7.500 1.600	(10912) aegid "BrD" and r aegid "BrD" and r 2.200 1.200	2002 2002 200	(31032) megid "BrD" and r megid "BrD" and r 2.300 1.300	(31042) eegid "BID" and resid 72 and name segid "BID" and resid 72 and name 2,200 1.200 1.200 peak 31042	(31052) segid 'BrD and segid 'BrD and 1.900 0.900	f (1622) emgid BrD and resid 110 a. (emgid BrD and resid 78 a. 2.100 2.400 pes.	egid BrD and egid BrD and 1.700 3.400	egid BrD and gid BrD and 700 1.800	mgid 'BrD and mgid 'BrD and .000 2.200	#914 'BrD and #914 'BrD and .200 4.200	emegid BrD and emegid BrD and 3.400 [6222]
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1.246	1.539	4.752	9.765	1.221	1.066		2,320	1.253	3.157	1.66	1.73	1.653	1.083	1.084	4.530	3					0.00	.62	0.67
1.599 ppeg	2.291 ppm2	2.190 ppm2	2.191 ppm2	1. 991 ppm	1.991 ppm2	\$.000 pom2	1.650 ppm2	1.646 ppm2	1.647 ppm2	4.164 ppm2	4.164 ppm2	5.146 ppm2	3.522 ppm2	3.669 ppm2	4.802 ppm2	1.646 ppm2			200		1.050 ppm2	1.057 ppm2	1.599 ppm2
0.52799E+03 ppm1	0.34161E+03 ppm1	0.120345+03 ppm1.	0.11\$35E+03 ppm1	0.15622R+03 ppm1	0.56980£+01 ppm1	0.601525.02 ppm1	0.32952E+03 ppm1	0.36117E+03 ppm1	0.13044E+03 ppm1	0.559136+02 ppm1	0.39252E+02 ppm3	0.32100K+02 ppm1	0.95501E+02 ppm1	0.86786E+02 ppm1	0.14301E+03 ppm1	0.17717E+03 ppm1	0.206958+03 pom3	0.61204K+02 pm1	0.89516E+02 ppm1		0.21908E-03 pgm1	0.209238+03 ppm1	. 62220K+02 ppm1
10000E-01 volume	0.10000E+01 Volume	0.10000E+01 VG ume	0.10000E+01 volume	.10000E-01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000K+01 volume	0.10000E-01 volume	0.10000K+01 volume	10000E+01 volume	0.10000£+01 volume	0.10000£+01 volume	0.100008+01 volume	10000E+01 volume	0.100008+01 volume (0.10000E+01 volume (0.10000E+01 volume c		0.10900£+01 volume o	0.16666E+81 volume 0	3.10000E+01 volume 0
Me KD24) 22 weight 0	HD11) Weight	HBV)	KB4) HG2))	ME HOZA) 12 weight o	HB1) HD14) we 1ght	#01 1 #01 1	HG2N) HBN J	HD24)	HG21) HG))	HG1V)	A MEN 11	KA)) KD16)	HB2 1) HB14)	HB1)) HD1()	e KA)) e KB2)) 2 veight 0.	HD14) HA 1)	HO1))	HG121)	HO 1) HD24)	HO))	HD1%) HO))	ND10) NA 1)	HD24) HD24) Veight (
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VO Lubes

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2.980 ppm2

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1.129

4.907 ppm2

0.34957E-02 ppm1

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0.10000E.01

1.320

4.510 ppm2

0.80809E+02 ppm1

2.788

3.000 ppm.

0.32594E+02 ppm3

2.799

4.755 ppm3

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5.099 ppm2

0.78869E+01 ppm1

volume

2.311

1.00 ppm2

0.91996E.02 ppm1

0.67300£+03 ppm3

volume

4.460

3.080 ppm2

0.147878+03 ppm1

volume

0.10000E+01

4.509 ppm2

0.18352E+03 ppm1

1.507

2.334 ppm2

0.46116E+02 ppm1

2.176

2.291 ppm2

0.90515E+02 ppm1

volume

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2.979 ppm2

0.16032E+03 ppm1

volume

2.571

5.347 ppm2

0.437138.02 ppm1

volume

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0.58134E+02 ppm1

volume

2.467

3.288 ppm2

0.18992K+02 ppm1

0.10000E+01 volume

3.321

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0.30644E+03 ppm1

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and resid 59 100 2.000	7.5			2.000	001d 36 001d 22 2.400	seid 56	3.3	resid 22 resid 43	meid 25 2.100		asid 49 1.500	neid 54 resid 57 1.900	2.000	eeid 63 1.800	1.500	estd 49	and 76	201.1 20 34 34 34	2.100	1.300	and resid is	001d 14 2.200	and resid 12 and resid 14	and resid 74
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	##914 3.500 1.500		(16412) #91d	4.700 (16492) eegid "	2.200 (16502)					6682)	((segid "B ASSI (16792) ((segid "B ((segid "B	2.700 {16842} eegid *B	2.200 (1688)	4.100 OR (16882) (1 #egid ((megid	(16892 aegid 2.200	(16902) segid B	(1693) segid segid 5.500	(16972) segid "B acgid "B	(1703) megid megid 2.400	(17072) segid 'BrD segid 'BrD 3.800	(17192) eegid "		(segid Bro (segid Bro (segid Bro 1.900 (segid Bro (segid Bro (segid Bro (segid Bro
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į		7.934	7.933	1.571	2.312	.63	1.434	3.200	3.206	1.897	2.540	7.827	006.6	1.652	6.022	2.367	6.998	1.140	3.149	2.883	2.884	2.605	1.571
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75	<u>.</u>	76 ppm2	77 ppm²	65 ppm2	74 ppm2	72 ppm2	72 ppm2	73 ppm2	23 ppm2	73 ppm2	70 ppm²	23 ppm2	36 ppm2	15 ppm2	70 ppm2	pbus 5	12 ppm2	19 ppm2	2 ppm2	. 2mdd 6:	2 ppm2	13 ppm2	4.999 ppm2
ŕ	;	3.276	7.0.0	4.165	3.374	3.572	3.572	3.872	3.672	. 1.573	3.670	3.673	4.606	3.818	3.670	5.146	3.522	3.669	3.522	3.669	3.522	3.522	• •
١	į	pdd 1	T Made	į	100	t and a	t mdd		ppm1	ppa 1	i de	pper	1		ppe	t equ			Ē	Ĩ.	II.	. 1	Ĩ.
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a toy		mnlov 1	m lov 1	m tov 1	wolume	volume	volume	un fox 1	an too 1	volume	volume	volum	volue	volum	volen	volume	volume	volume	volume	volume	volume	volume	wolum
0.10000E+01.volume		0.10000K+01 volume	0.10000K+01 volume	0.10000E+01 volume	0.100005+01	0.10000E+01	0.100005+01	0.10000K+01 volume	0.10000E+01 volume	0.10000E+01	0.10000E+01	0.100608+01 volume	0.10000R+01 volume	0.10000E+01 volume	0.100002+01 volume	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.100006+01	0.10000E+01	0.100008+01	0.10000K+01 volume
HB1 1) HG14) veight		MB2))	HDI)	KG2V)	K83 >)	HB1))	KB1)) KG2))	HB2	HBI)) HBI)	KB2 1) HB2 1)	HB1)) HG2))	KD4)	# 19 m	HD14) Weight	HB1)) HZ))	KG 1)	HB2)) KDN)	KDI))	KB2 }) HD1 })	KB1))	HB2)) HB1))	NB2) NB1) weight	HA)) HG24) Veight HB1))
and name and name peak 15012	d name	peak 15032 and name	peak 15042	and name peak 15052	and name and name peak 15092	and name and name peak 15162	and name and name peak 15192	and name and name peak 18402	said 82 and name is said 99 and name is 2.100 peak 15412 a	reid 82 and name P reid 163 and name P 1.800 peak 15552 v	and 107 and name is 103 and name is 2.400 peak 15593	said 107 and name 1 said 107 and name 1 1.200 peak 15712	and name and name pesk 15812	and name and name pask 15882	11d 82 and name 11d 107 and name 1.700 peak 15932	and name and name peak 16052	and name and name peak 16062	and name and name peak 16112	and name and name peak 16122	and name and name peak 16132	and name and name peak 16152	and name and name pask 16162	0.000 0.000 0.000 0.000
	and a	* 1	- 0 - 4 - 1		4 4 4	2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	2 and 2 pask 1	4 4 4	4 4 4	2 G O	200	200 7	114	8 8 4	2 and 07 and 0 peak 1	344	e end	111	Per sha	\$ \$ \$ \$	334	\$ \$ \$ \$	
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b . and .	77 77	4.500	- pue	3.20	BrD and r	gid "BrD " and : gid "BrD " and : 000 4.000 5192)	* * * * * * * * * * * * * * * * * * *	2 a a	rD . and r 2.100	3.400 in	pu	200 and	id BrD and resid	9 00 00	0 * and r	pue 000	and 200	pu oo	100 I	0 and r	2 pue	2 and r	2.600 2.600 0 and r
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0.99455E+02

0.10000E+01 volume

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HH2 !!

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1.127 ppm2

0.22025E+02 ppm1

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4.803

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-	1.1	1.774	4.907	7.903	7.706	7.263	7.063	4.452	4.020	3.654		2.304	1.707		4.44	7.699	1.662	2.403		1.327	9		2.165
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0.12013E.03 pres		0.248068+02	0.61169E+01	0.459968+02	0.32265E+03	0.48682E+03	0.159808+03	0.116338+03	0.510048+02	0.94735E+02	0.53516E+02	0.422468	0.211\$5K+02	0 26579E.02	0.228896+02	0.302738+02	0.74474E+02	0.289306+03		0.108578+02	0.166216.02		0.47142E+02 ppm1
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HB1))		HB2 1) HE')	44 8	HG24)	HO24) HD4)	HG24) HDA)	HEN)	HG1))	HG1))	HO1))	HG2)) HA))	HD1))	KD2 1)	KB1))	KB2)	HDV)	HO1))	K01))	KG2 ()	HG2 1) HD14)	MGZ)) MD14) weight	191 101 101 101 101 101 101 101 101 101	HO1)) HB1))
d name	and name	and name and name peak 17452	and name and name peak 17502	and name and name peak 17562	and name and name peak 17572	and name and name peak 17632	and name and name peak 17642	and name and name peak 17712	and name and name and name 17732	and name and name peak 17742	and name and name and name peak 17762 v	and name and name peak 17782	and name and name peak 17903	and name and name peak 17952	and name and name peak 17962	and name and name peak 17962	and name and name peak 18012	iid 59 and name iid 59 and name 1.700 peak 18052	* P	d name 18102	eid 59 and name isid 22 and name in 1.400 peak 18112 v	P 20 P	d name d name 18122
554	- 2	111	111	2 2 4	end Ask	2 5 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	3 4 4	444	114	444	2 2 4	a a a	P 2 2 2	354	111	3 5 4	P P P P P P P P P P P P P P P P P P P	\$ \$	S A A A	3 3 4	P P	334
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1554	OR (17372) ((eegid 'BrD ' and re (eegid 'BrD ' and re	- ig	3 3		8		ASS: -	, , , , , , , , , , , , , , , , , , ,	ABBI 3		ABSI A		, 1984	Year C	== 8	1894		(eegid	===			OR (10112) (meg1d (meg1d	Assi (

1.994		3.34	3.101	1.68	2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2	7.852	4.026	4.427	3.537	3.003	1.906	2.634	0.676	1.425	· •	3	1.910	1.0	1.986
3.523 ppm2	2.762 ppm3	2.762 ppm2	2.783 ppm2	2.762 ppm2	2.782 ppm2	3.226 ppm2	2.634 ppm2	2.634 ppm2	2.634 ppm2	2.634 ppm2	2.634 ppm2	2.634 pped	2.634 ppm2	2.634 ppm2	1	2.63 ppm2	2.435 ppm2	2.635 ppm2	2.634 ppm2
0.23045E+02 pm1	0.18338E+03 ppm1	0.50813E+02 ppm1	0.11214E-03 ppm1	0.15609E+03 ppm1	0.41055E.03 ppm1 0.27206E.03 ppm3	5	0.103D48+03 ppm1	0.51911E+02 ppm1	0.13576R+03 ppm1	0.11929E+03 ppm1	0.11115E+02 ppm1	0.10446E+04 ppm1	0.60941E+01 ppm1	0.277975+03 ppm1			0.79723E+01 ppm1	0.40230E+02 ppm3	0.225788+03 ppm1
0.10000E.01 volume	0.10000£.61 volume	0.10000E.01 volume	0.10000E+01 volume	0.100508+01 volume	0.10000E+01 volume 0.10000E+01 volume	0.100006.01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000E.01 volume	0.10000E.01 volume	0.10060E.01 volume	0.10000E+01 volume	0.10000E+01 volume	0.100008-01-man	0.10000g+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.100008+01 volume
resid 75 and name HG1)) resid 113 and name HB4) 1.600 pesk 18142 weight	resid 35 and name HEt) resid 60 and name HB1 }} 2.000 peak 18282 weight	ceid 35 and name 2.100 peak 18302	resid 35 and resid 35 and 2.200 pask 3	reeid 35 2.000	1.400 peak 1932 c	0.500 0.500 0.500 0.500	ceid 75 and name ceid 17 and name 3.200 peak 18542	esid 75 and name esid 110 and name 2.100 peak 18642	2.100	2.200	esid 75 esid 75 1.800 pe	resid 75 and name HBt) resid 75 and name HB2)) 2.400 pask 18732 weight	resid 75 and name HEW) resid 76 and name HD2v) 0.600 peak 18762 weight	resid 75 resid 14 1.700 pe	resid 75 and name HE%) resid 14 and name HD2%) Feeid 15 and name HE%) 2.000 peak 18782 weight	resid 75 reeld 116 1.900 pr	resid 15 and name HEt) resid 116 and name HG11)} 0.900 pesk 18862 weight	reeld 75 and name MEV) reeld 59 and name MEV) 2.000 peak 18872 weight	resid 75 and name MEA) resid 113 and name MBA) 1.800 peak 18882 weight resid 75 and name MEA)
({ aegid "BrD " and eegid "BrD " and 1.900 3.800 ASSI [1828]	eagid 'BrD and segid 'BrD and 2.800 2.000 [18102]	aegid BrD and aegid BrD and 3.400 2.900 e302}	ASS (89914 MT) - end (89914 BT)	megid "BrD " and 2,600 2.000 {18362}	2.400 1.400 (10102) eegid BrD and eegid BrD and 2.500 1.600	[18632] segid "BrD" and segid "BrD" and 5.000 5.000 5.000 segid "BrD" and segid "BrD" and	Assi (18542) (segid "BrD " and i (segid "BrD " and i 3.000 2.200 Assi (18642)	eegid BrD and segid BrD and 3.400 2.900 [1862]	(segid "BrD sand i ((segid "BrD sand i 2.900 2.100 ASSI {18622}	(segid 'BrD and r ({ segid 'BrD and r 3.000 2.200 ASSI (18722)	megid 'BrD ' and begid 'BrD ' and 3.700 3.400 (18732)	megid 'BrD and 2.100 2.100 (18762)	segid 'BrD and segid 'BrD and 4.900 4.900	segid BrD snd aegid BrD and 2.600 1.700	megid BrD and megid BrD and (1972) megid BrD and megid BrD and megid BrD and	ABE [18812] [megid "BTD" and a [{ megid "BTD" and a 3.400 3.200	megid BrD and	segid 'BrD and segid 'BrD and 3.500 3.100	megid "BrD" and a segid "BrD" and a 1.800 (1882) megid "BrD" and a megid "BrD" and a

bae " Grd" biges)	1.800 2.000 OR (19492) (eegid 'BID' end (secid 'BID' end	ASSI (19502) (emgid "BrD " and (emgid "BrD " end 2.700 1.800	A881 (19522) [eegid BrD end {{ eegid BrD end 2.800 2.000	ASSI (19552) (eegid '8rD * and (eegid '8rD * and 2.500 1.600	OR {19552} [segid 'BrD * and ((segid 'BrD * and ASB1 [19572]	{ megid BrD and { megid BrD and } 3.600 }.200	(segid BrD = end ((segid BrD = end 2.800 3.000 AMM (19933)	((megid "MID " and ((megid "BID " and 3.100 3.400 ASSI (19642)	(eegid 'BrD ' and (eegid 'BrD ' and 2.200 ASSI [1962] (eegid 'BrD ' and (eegid 'BrD ' and	(segid BrD and 2.300 ASSI (19672)	2.500 1.600 ASSI [19692] (eegid BrD " and ({ eegid BrD " and	3.100 2.400 ASSI [19702] eegid 'BrD and { eegid 'BrD and { eegid 'BrD and	ASB1 [19752] (eegid "BrD and (f eegid "BrD and 3.000 2.200	ASSI [19772] { aegid "BrD " and ({ aegid "BrD " and 1.500 1.100	ASSI [19792] ((megid "BrD " and ((megid "BrD " and 2.600 1.700	ASS1 (19802) ({ angld "BrD " and (angld "BrD " and 2.700 1.800	ASSI (19812) ([segid "BrD " and (segid "BrD " end 1.200 2.600	ASSI {19822} (1 eegid "BrD " and (eegid "BrD " and 2.800 2.000	ASSI (19812) ((segid "BrD " end ((segid "BrD " and 2.600 2.000	(eegid 'BrD ' and (eegid 'BrD ' and (eegid 'BrD ' and 2.600 1.700	(19882) segid "B aegid "B	A581 {19902} ({ segid "BrD " and ({ segid "BrD " and (1 segid "BrD " and 1,400 2.800	A881 [19912]
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2.250	2.199	2.44	4.289	5.444	7.83	5.428	7,417	2.735	2.646		0.799	1.1	2.033	1.790	1.632	2.843	1.581	3.427	3.134	4.582	7.803	3.663	
2.636 ppm2	2.635 ppez	2.636 ppm2	2.847 ppm2	2.842 ppm2	\$.001 ppm2	\$.001 ppm2	5.847 pm2	5.544 ppm2	5.544 ppm2		5.544 ppm2	1.697 ppen2	1.697 ppm2	1.697 ppm2	2.289 ppm2	2.289 ppm2	2.289 ppm2	2.289 ppm2	2.289 ppm2	2.289 ppm2	2.289 ppm2	2.092 ppm2	
0.37764E+03 ppm1	0.35880E+03 ppm1	0.292556+02		0.28694E+02 ppm1	0.94899E-02 ppm1	0.15610£+03		0.12256E+03 ppm1	0.973015+02 ppm1		0.423196+02 ppm1	0.31463E.01 ppm1	0.60793E+02 ppm1	0.12011&+01 ppm1	0.680196+02	0.481698+02 ppml	0.37768E+03 ppm1	0.30400E+03 ppm1	0.14651E+02 ppm1	0.871838+02 ppm1	0.442238+02 ppm1	0.66817E+02 ppm1	
0.10000E+01 volume	0.109008+01 volume	0.10000E+01 volume	0.10000E-01 volume 0.60763E-02	0.10000E+01 volume	0.10000E+01 volume	0.10000£+01 volume	0.100008+01 volume 0.582348*02	0.10000E+01 volume	0.100008+01 volume		0.10000E+01 volume 0.42319E+02 ppml 0.10000E+01 volume 0.3597E+02 ppml	0.10000E+01 volume 0.31463E+01	0.10000E+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000K+01 volume	0.10000\$+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000K+01 volume	
and name HG)) peak 18892 weight	seid 75 and name HEN) Reid 115 and name HB1)) 1.600 peak 18902 weight	and name HEt) and name HB1)) peak 18912 weight	and name and name peak 18952	and name and name peak 18992	and name HA)) and name HZ)) peak 19072 weight	and news HA }) and news HA)} peak 19092 weight	and name HA and name HEL peak 19172 weight	and name HA)) and name HGI)) peak 19182 weight	and hame and ness peak 19192	and name NA)) and name HB2)) and name NA)) and name NA))	and name and name peak 19212	and name and name peak 19242	and name and name peak 19272	and name MB%) and name HB)} peak 19282 weight	and name and name peak 19312	and name HB%) and neme HB1)) peak 19352 weight	and name KB4) and name KB1)) peak 19362 weight	and name HB%) and name HG1)) peek 19372 weight	and name HB4) and name HB2)} peak 19382 weight	and name HB1) and name HA)} peak 19392 weight	and news HBt) and nems HEt) peak 19422 weight	and name HBt) and name HB2)) peak 19482 weight	
1.400		1. 800	2.300	eaid 57	esid 34 2.400	2.000	2.200	2. 100	2.400	:: ::	2.00 e1d 43 1.90	eid 43 0.100	2.200	2.200	ee1d 31 2.300	2.100	eid 31 eid 28 1.400	eeid 31 eeid 35 1.600	16 biss	meid 31 2.400	eid 31 2.000	asid 76	
((megad "BrD * 2.400 1	(segid "BrD " and r ((segid "BrD " and r 2,500 1,600	(segid 'BrD ' and r (segid 'BrD ' and r 3,700 3,400	Asst [18952] [{ segid 'BrD ' and [{ segid 'BrD ' and 3.200 2.600		(eegid 'BrD ' and r (eegid 'BrD ' and r 1.100 2.400		(segid BrD . (segid BrD .) . 100 . 2	((megid "BrD " (megid "BrD ") 2.900 2.1	((segid 'BID' and re ((segid 'BID' and re 3.100 2.400 OR (19192)	((megid BrD : ASSI (19202) ((megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (megid BrD : (3.500 3.1 ASSI {19212} (megid "BED " ((megid "BED " 3.600 3.2	ASSI (19242) (megid "BrD " (megid "BrD " 5.400 5.	ASSI (19272) (segid BrD (segid BrD) 1,300 2.	Assi (19282) (segid BrD * (segid BrD * 3.000 2.	(segid "BID " and r (segid "BID " and r 3.200 2.600		(segid "BrD " and r ((segid "BrD " and r 2.400 1.400		(segid BrD () () () () () () () () () ((segid BrD (segid BrD)	(segid 'BrD ' and r (segid 'BrD ' end r 3.500 3.100	(eegid BrD (eegid BrD) 3.300 3.40	

2.564	2.507	9	1.763		1.43	.30	2.327	7.803	7.781	7.259	\$.005	**	3.63	2.784	7.901	1.77.6	7.073	7,289	4.850	1.922	1.222	3.670
2.092 ppm2	2.092 ppm2		2.092 ppm2		3.093 ppm2	1.500 ppm2	4.656 ppm2	2.190 ppm2	2.190 ppm2	2.190 ppm2	2.190 ppm2	1.190 ppm2	2.190 ppm2	2.092 ppm2	4.459 ppm2	4.459 ppm2	4.457 ppm2	4.459 ppm2	6.458 ppm2	4.458 ppm2	4.903 ppm2	4.303 ppm2
1.15977£+03 ppm1	0.21416£+03 ppm1	0.15327E+03 ppm1	0.32487E+03 ppm1		0.35020&+02 ppm1	0.16661E-03 ppm1	.95067E+02 ppml	.652408+03 ppm1	0.50164E+03 ppm1	0.360385-03 ppm1	.92786K+02 ppml	10441E+03 ppm1	0.10256£•03 ppm1	.45000\$+02 ppm1	.26558E+03 ppm1	0.214676+03 pgm1	0.713958+02 ppm1	.15492E+03	0.16591E+03 ppm1	.24667E+03 ppm1	.15801E+02 ppm1	0.48759E+02 pj.ml.
.logoog.ol volume o	0.10000E+01 volume o	0.10000K+01 volume 0	0.10000£.01 volume 0		0.10000E+01 volume 0	0.10000£+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	.10000£+01 volume 0	0.100668.01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000\$+01 volume 0	0.10000E+01 volume 0	0.10000£.01 volume 0	0.100008.01 volume 0	0.10000K+01 volume 0.	0.10000E+01 volumm 0	0.10000E+01 volume 0	0.10000E+01 volume 0.	0.10000E+01 volume 0
and name HB2 1) and name HB2 1) ask 19492 waight 0 and name HB4)	MBN) MB2))	HB.)	and name HBt and name HB2 }	neme HB1)	and name HB%) and name MG2%) sak 19572 weight 0	and name HD2%) and name HA)) ask 19582 weight 0	MA 1) HQ1)) weight	HB4) H2)) weight	I name HB%) I name HB%) 19652 weight 0	HBA) HDA) weight	HB.)	HB)	HB4) HG1))	KB) HBI))	KZ))	HE L	KE)	HD.)	d name NA)} d name NA)) 19832 weight 0.	HA 1) HB2 1)	HG26) Weight	1200 HB1 1)
reeld 76 and 2.000 peak 1	4 4 4	resid 76 and name resid 77 and name 2.000 peek 19522	resid 76 and resid 51 and 1.600 peak 1	resid 76 and resid 51 and	Δ.	resid 73 and Testd 6s and 7.000 peak 3	resid 30 and name resid 80 and name 2.400 peak 19632	resid 99 and name resid 34 and name 2.300 peak 19642	esid 99 and esid 34 and 1.300 peak	eeid 99 and eeid 82 and 1.600 peak 1	resid 85 and name 2.400 peek 19692	resid 100 and name 2.200 peak 19702	resid 39 and name resid 103 and name 2.200 pask 19752	reeid 76 and name reeid 79 and name 2.000 peak 19772	resid 34 and name resid 34 and name 1.700 peak 19792	resid 34 and name resid 34 and neme 1.800 peak 19802	resid 99 and name resid 82 and name 2.300 peek 19812	resid 99 and name resid 82 and name 2.000 peak 19822	resid 99 and resid 100 and 2,000 peak 1	resid 99 and name resid 101 and name 1.700 peak 19842	resid 113 and name resid 110 and name 1.900 peak 19882	resid 113 and 1 resid 112 and 1 2.100 peak 11
2.000 end	[19502] eegid "BrD " and r eegid "BrD " and r 2.700 1.800	170 • and 2.000	9r0 and 9r0 and 1.600	Brb . and	BrO * and 3.200	rrb and rrb and 3.000	and and and a. 400	BrD and BrD end 2.200	eegid 'BrD and r eegid 'BrD and r 2,300 1,300	eegid "BrD " and r eegid "BrD " and r 2.500 1.600	egid 'BrD " and r egid 'BrD " and r .100 2.400	egid BrD and r egid BrD and r .000 2.200	eegid BrD and r eegid BrD and r 3.000 2.200	eegid "BrD and r eegid "BrD and r 1.500 3.100	aegid 'BrD and r aegid 'BrD and r 2.600 1.700	megid SrD and r megid SrD and r 2.700 1.800	BrD and 2.600	2.000	aegid "BrD" and r megid "BrD" and r 2.600 2.000 (19842)	Bro and Bro and		megid BrD and r megid BrD and r 3.400 2.900 [19912]
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0.44605R+02 ppm1	O.84488E+02	0.185726+02	0.6040511.02	0.066366.03	0.14101E+02	0.472596+03	0.33630K.03	0.76060E+02	0.867176	0.27619E	0.100986.03	0.461348+02	0.25743E+03	0.846108+01	0.674878+02	0.427175.03	0.1367464	0.513675.02	0.263546+03	0.135965	0.750858+02		0.44748E.03
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0.100	0.100	0.100	9.100	0.10000E+	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.1000	0.1000	0.1000	0.1000	.1000	0.10000£+01	0.10000\$+01	6.10000E+01	0.100002+01	0.100006+01		. 100
HA))	THE STATE	HD16)	HB4) HB1))	HB) HG))	HB1) HD21)	HBY) HDIN)	HA)) HOIN) Height	KB)) KD14) weight	HA)) HD14)	HG1() HE1) weight	HG21) HB 1) weight	HG24) HB1))	HG26) HB2 }}	HB2))	HB))	HD2)) Weight	KA 1) K01))		- 4	MO24) MD1))	- 4		, 11
112	223	112	name HB name HB 19992 we	883	223	# # S	183	112	193	2 2 C	2 E B C E B	2 E E	M KB2	1	# # Z	1 F F F	\$ 2 2 2	ME HG2N)	M HO1)	2 E E E	H02V)		
said 113 and name is a 110 and name 12.000 peak 19912	resid 113 and name H resid 14 and name H 2.400 peak 19922 w	resid 113 and name H resid 115 and name H 1.500 peak 19962 w	aid 113 and name sid 14 and name 2.200 peak 19992	resid 113 and name resid 14 and name 2.400 peak 20032	resid 113 and name H resid 15 and name H 1.300 peak 20042 w	resid 113 and name H resid 115 and name H 1.400 peak 20052 w	reid 110 and name Peatd 115 and name P	resid 17 and name H resid 115 and name H 2.300 peak 20192 w	resid 17 and name resid 21 and name 0.900 peak 20212	said 17 and name H said 75 and name H 1.700 peak 20242 w	resid 17 and name H resid 21 and name H 2.200 peak 20252 a	resid 17 and name H resid 115 and name H 2.000 peak 20272 a	end 10 and name Head 109 and name H	resid 17 and name resid 10 and name 0.900 peak 20302	and name and name peak 20312	and name and name peak 20332	and name and name peek 20382	and name and name peak 20532	resid 41 and name H resid 39 and name H 1,700 peak 20542 w	and name and name peak 20562	and name and name pack 20572	and name	and name
11 8 F	3 2 8	3 2 3	resid 113 and resid 14 and 2.200 peak 1	3 2 8	228	110	310	8 2 2	822	228	218	228	2028	2.28	2 A 8	***	::8	222	228	228	118	338	
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7 T T T	3 5 18 9	- B	-=			8	÷-	ASS1 (- 198v	ABBI (- 5		(megid "B ((megid "B 2,600	, , , ,	2 2 2		22	5	(megid '8 (megid '8 2.600			22	# 2 2 2 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
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;		7.036	7.920									È	7.518	7.026	1,327	!	0.676	2.187	3.907	1.36	4.287	4.783	4.659	7.706
7 66		1.648 ppm2	1.651 ppm2	1. 648			2. 63 ppm		6.603 poss	1.05				1.795 ppm2	1.979 ppm2	:	2.979 ppm2	1.785 ppm2	1.786 ppm2	1.797 ppe2	1.794 ppm2	0.760 ppm3	1.056 ppm2	1.056 ppm2
0.175308-03 ppm1		0.13726E.03 ppm1	0.69485E+02 ppm1	0.55839E+02 pgm1	0.12367E+03 ppm.1	0.11109ff.01 ppm1	0.97465E+02 ppm1	0.11102E+03 ppm1	0.55703E+02 ppm1	0.10489E+04 ppm1	0.478288.02 promi			Catalogue of post	0.35593E+02 ppm1		0.11302E+02 ppm1	0.436748+02 ppml	0.11856E+02 ppm1	0.21023K+03 pgm1	48910E-62 ppm1	0.12812E+03 ppm1	64039E+02 ppm1	5277eE.02 ppm1
0.19000E+01 volume			0.10000E+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.18080E+81 volume	0.10000E+01 volume	3.10000£+01 volume	0.10000£+01 volume	0.10000E+01 volume	0.10000E+01 volume	0.10000E-01			. 10000E+01 volume		.10000E+01 volume (10000E-01 volume	0.10000£+01 volume 0	0.10000E+01 volume 0	.10000£+01 volume 0	0.1000E+01 volume 0	0.10000E+01 volume 0	0.100005.01 volume 0
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1.402	5.359	1.785	4.867	1.483	7.533	7.014	1.317	4.541	4.059	3.001	9.676	4.62	3.557	3.516	\$	3.678	3.527	7.006	1.5	3	
2.142 ppm2	1.401 ppm2	1.401 ppm2	3.867 ppm2	2.144 ppm2	0.911 ppm2	0.911 ppm2	2.390 ppm2	0.415 ppm2	1.056 ppm2	1.056 ppm2	1.056 ppm2	1.057 ppm2	\$.294 ppm2	2.437 ppm2	2.437 ppm2	1.649 ppm2	1.669 ppm2	1.648 ppm2	4.311 ppm2	900	
702878+03 ppm1		0.26555K+02 ppm.l 0.23696K+03 ppm.l	0.41356E:02 ppm1	0.21633E.02 ppm1	0.77851E+02 ppm1	32246E+02 ppm1	0.94731E+01 ppm1	0.52852E+02 ppm1	0.21\$65E+02 ppm1	0.32596E+02 ppm1	0.41978E+02 ppml	0.49516E+02 ppm1	0.61304E+02 ppm1	.514218.02 ppm1	.29636K+03 ppm1	0.38413E-02 ppm1	0.1223&£+03 ppm1	0.76917£+02 ppm1	0.84277E-02 ppm1	0.#4034K+03 ppm1	
Volume 0.	volume	vol use	vol use	volume	volume	volume o.	volume	volume	volume	volume	volume	vol ume	volume	vol Ca	volume 0	volume	volume	volume		volume	
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(23732) segid 'BrD sand segid 'BrD sand 2,200 1,200 23732) segid 'BrD and segid 'BrD and (23762)	egid 'BrD and 2.400 2.802) egid 'BrD and egid 'BrD and end 2.600	[23842] segid 'BrD and segid 'BrD and 2.600 1.700	eegid "BrD " and a 3.500 3.500 3.500	segid 'BrD and 1.800 1.800 (21972)	##91d BrD and r ##91d BrD and r 3.200 2.400 [23982]	megid "BrD " and a megid "BrD " and a 3.700 3.400 [24022]	megid "BrD " and a megid "BrD " and a 4.500 4.500 (24032)	segid 'BrD ' and segid 'BrD ' and 3.400 2.900 {24203}	segid "BrD " and a segid "BrD " and a 3.900 3.900 [34232]	11d *BrD * and 11d *BrD * and 100 3.400	eegid 'BrD " and s eegid 'BrD " and s 3.500 3.100 {24273}	11d "BrD " and 11d "BrD " and 100 2.900 302}	segid 'BrD ' and r segid 'BrD ' and r 3.300 2.700 {24452}	segid "BrD " and r segid "BrD " and r 3.400 2.900 [24462]	segid 'BrD * and r segid 'BrD * and r 2.500 2.500 [24482]	megid 'BrD and megid 'BrD and 3.600 3.200 [24512]	segid 'BrD and r segid 'BrD and r 2.900 2.100 [24542]	segid "BrD " and 31.200 2.600 [24662]	2.400	61.5 2.60 2.60	16 'BrD ' and 14 'BrD ' and
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Ξ))))	1884	ASSI	1884	ASSI	ASSI	1887 	ASSI 1.0	ASSI	1554 -	YS61	- Y881	Assi)) Y881	YSB1	1884	1884	1884	7 1897	7 188V	, A881	, 1881 , .) 198V	
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7.487	7.469	1.654	1.888	1.886	7.519	7.511	1.746	1.746	1.323		4.647	1.498	1.312	0.902	7.638			*	3.475	4.525	4.932	1.311	1.311	
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-	2.191	2.191	3.124	3.06	3.406	1.648	1.648	2.336	2.336		1.646	2.336	1,205	1.205	1.599		1.59	4.261	4.361	1.536	2.536	2.536	4. 804	
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2 weight	# KE) 2 weight	# HD1)) # HD1%) 2 veight	# HG1))	# H02)) # H01))	HD))	HO12)) HD1)	# HG12)) # HG2%) 2 weight	# H011) # H026) 2 weight	# HG11)) # HD24) 2 weight	# HO11)	# KG12))	M HG1)) M HG2))	# KD14)	M HD14)	M HO2V)	Me HG20) Me HZ)) 32 weight	HOZV)	E KA	ne KA)) ne HB1))	2 E E	4 E E	M HB 1)	HA HO10)	- 5
peak 24782	and name and name l	and name and name peak 24442	reald 23 and name reald 19 and name 1.700 peak 24682	reald 21 and name H resid 19 and name H 1.600 peak 24892 w	reald 21 and name resid 106 and name 1.400 peak 25012	resid 21 and name H resid 106 and name H 1.200 peak 25022 a	resid 21 and name resid 17 and name 2.000 peak 25072	nd nen nd nen sk 2506	nd nee	and bru	ind near	and near and near	and nas and nas	and near and near	and named 252	and named na	and par and par 253	resid 101 and name resid 100 and name 2.100 peak 25322	reald 101 and hame reald 100 and hame 2.400 peak 25332	aid 101 and name HB) aid 30 and name HB2) 2.300 peak 25342 weight	14 101 and name HB)) 14 10 and name HB1)) 2.100 peek 25352 weight	eid 101 and name laid 102 and hame 2.000 peak 25362	1 96 and name HA 1) 1 102 and name HD11) 400 peak 25183 weight	and name
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1.970 1.410 7.789 7. 63 2.102 5.41 7.73 4.933 7.093 7.778 4.532 4.932 3.069 3.012 2.157 0.676 4.511 4.569 7.529 4.533 2.206 2.206 P. 7.79 . 40 1.697 ppm2 4.015 ppm2 2.338 ppm2 ppm2 Ž 1.549 ppm2 1.599 ppm2 1.599 ppm2 1.549 ppm2 1.155 ppm2 4.013 ppm2 3.620 ppm2 3.916 ppm2 3.670 ppm2 3.620 ppm2 3.917 ppm2 1.551 ppm2 1.599 ppm2 1.599 ppm2 1.154 ppm2 1.254 ppm2 1.251 pped 1.155 ppm2 1.184 ppm2 4.804 1.804 0.10000E+01 volume 0.66772E+02 ppm1 ppm1 ğ ã ã ã i edd ptm1 ppm Ĩ. Ĭ ě ě T dd E M Ĭ ă, 1 ě ă Ž 0.30316E+02 ppml 0.62906E+02 ppm1 0.45042E+03 0.38225E+02 0.220348+03 O.BILIBEROL volume volume volume volume volume volume 0.10000E+01 volume volume vol une volume volume volume volume 0.10000E+01 volume 0.10000E+01 volume 0.100008.D1 volume valume volume volume Volume. 0.10000E+01 0.10000E+01 0.10000E+01 0.10000E+01 0.10000E+01 0.10000E+01 | 15.25 | 10.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 id '8ED' and reald 110 and name ED11)

(d '8ED' and reald 10c and name ED11)

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2 22				161) (141)					HBI))		weight 0 HB2)) HG24)	~~"				MD2 1) HB2 1)	HD2)) NB)) weight o	KD2 11 KA 11 weight 0	NG)) HG14) weight o		HB1)) HG1N)	HA))
	peak 26702 w and name H	d name H		and name H	d name K	0.200 peak 26952 w resid 112 and neme H	2.100 peak 26962 w sid 61 and name H sid 58 and name M	2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	d name H	200	and name H	d name H	resid 100 and name H resid 101 and name H	and 100 and name H said 99 and name H 2.100 peek 27112 w	aid 80 and name H 2.400 peak 27142 w	and name H and name H peak 27172 w	and hame H and name H posk 27192 v	and name K and name K peak 27203 v	and name H and name H peak 27323 w	and name H and name H peak 27342 w	and name K and name K peak 27352 w	
2 12	5 % E	1.700 peak 26752 resid 86 and name resid 87 and name	800 peek 2 36 and 57 and	2.000 peak 2 aid 37 and sid 54 and	1.500 peak 26922 visit 37 and name lead 36 and name	200 pesk	100 Per	2.200 peak 26972 seld 89 and name	1.600 peak 27022 said 89 and name	2.200 peak 27032 sid 100 and name	reeld 100 an	resid 100 and name resid 101 and hams 1.500 pask 27092	1 100 en	resid 100 an resid 99 an	4 4 6 6 4	1.400 pask	2.100 pask	526	2001	aid SS an aid 34 an 2.200 peak	58 Peak	2.000 peak 3
2 22		nd resid	nd resid 36	- 55	2.2	nd resid	2.2	2.2	2 2				nd resid	7.7	2.2	2.5	2 2	nd resid to	nd resid \$6 nd resid 81 0 2.100 p	nd resid \$5 nd resid 34 0 2.200	nd resid \$5 nd resid 81 0 1.600	
ero and srp and srp and	3.700 3.400 (26752) eegid 'BrD and eegid 'BrD and	2.600 1.700 [26872] segid 8rD and a	2.700 1.800 [26902] segid 'BrD' and segid 'BrD' and	922) id '9rD * and id '8rD * and	4.000 4.000 (26952) eegid BrD and segid BrD and	5.300 5.300 5.300 5.300 5.300 5.300 5.300 5.300 5.300 5.300 5.300	400 2.900 6972) gid 'BrD * and	17022 2.200 17022 2.200 1914 BrD and 1914 BrD and	14 H	(27082) (megid 'BrD ' and :	ous 4.000 gid 'BrD " and gid 'BrD " and	131 {27092} ((meg1d "BrD " end ((meg1d "BrD " and 4.000 4.000	27102} egid "BrD " and r egid "BrD " and r .700 1.800	112) 1d BrD and id BrD and 30 2.900	1142) 114 "BrD " and 1 114 "BrD " and 1	egid BrD and a	(27192) megid BrD and megid BrD and 3.400 2.900	9314 'BrD ' and egid 'BrD ' and egid 'BrD ' and	314 "BrD " and 1 314 "BrD " and 1 100 2.900	(27342) megid "BrD " and megid "BrD " and 3.300 2.700	ASSI [27362] ((megid BrD " and re. (megid BrD " and re. 3,900 3,800	BrD and BrD and 3.100
(26703) (26703) (magid 'BrD	1.700 [(26752) [eegid *B (eegid *B	2.600 [26872 (megid (megid	2.700 1 (26902) (eegid 'B	1 (26922 (segid (segid	4.000 [(36952 (segid (segid	(26962) megid "	. .			(27062) (eegid "	4.000 OR (27062) ((segid (segid		_ , , ,	_ , , ,						(megid Bri (megid Bri) 3.300	1 (27362 9 9 14 3 . 900	(eegid 'BrD (eegid 'BrD 3.800 ; (eegid 'BrD (eegid 'BrD
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7.493	1.914	1.918	1.976	5.160	2.662	2.176	1.906	1.140	4.427	3.508	1.662	1.710	1.637	1.078	0.6	1.237	4.818	1.200	1.263	1.149	4.679	\$.03
• ppm2	4 ppm2	• ppm2	4 ppm2	1.401 ppm2	1. ppm2	1.401 ppm2	1.401 ppm2	1.401 ppm2	1 ppm2	1 ppm2	1 ppm2	1.401 ppm2	1.401 ppm2	9 ppm2	1.399 ppm2	1.199 ppm2	1.501 ppm2	2 ppm2	ppm2	2.409 ppm2	5 ppm2	3.127 ppm2
1.254	1.254	1.154	1.154	1.40	1.401	1.40	1.40	1.40	1.401	1.401	1.401	1.40	1.40	1.399	1.1	1.13	1.50	3.433	2.409	3.4	2.519	3.5
184	2 PP#1	ppm 1	ppm)	2 ppm1	2 ppm1	2 9081) pps	ppm1	2 9981	2	2 ppm1		agg c	o ppm1	1	Ppm1	3 ppm1	2 ppm1	i app	2 ppm1	1	1 404 1
0.526416+02	0.30456E+02	0.561805+02	0.406305+0	0.13762E+02	79045E+0	0.258456+0	0.22212E+03	0.455788+03	0.761948+03	0.79386E+0	0.544006+02	0.240612+03	0.937966+03	0.391596+0	.55118E-01	0.13707E+04	0.60749E+03	0.11059E+02	0.35446E+02	0.651258+02	0.56609E+0	0.32\$72£+01 ppml
	4		volume 0.	g	volume 0.	•		9		volume 0.	valume 0.		,	volume 0.		volume 0.	9	volume 0.	volume 0.	Ĭ	volume 0.	•
0.10000E+01 volum	16.01 vol	8.01 volum		E-01 volum		E.Di vol	E-01 volum	Of. 01 volue	M.01 volum			0.10000K+01 volum	0.10000E+01 volus		08+01 vol		28+01 volum	08.01 VO		E-01 vol		0.10000E.01 volum
	0.100005.01	0.100008.01	0.10000E+01	0.10000E+01	0.160002+01	0.100002+01	0.10000E+01	0.10000[.01	0.100006.01	0.100005+01	0.100005+01	0.1000	0.1000	0.10000E+01	0.100008+01	0 . 100006+01	0.100008+01	0.100008.01	0.100005+01	0.100006+01	0.10000E+01	
HOZV) HB1))	H021) H011)	HD16) HG11)	HD14) HB4)	HG24) HA)) veight	HG26) HB3))	HB1))	HG11))	HO24) HD14)	HD10)	HD11) HO1))	KB1) KB2))	HD14) HO11))	HD14) HG12))	HB2))	HD1V) HD2V)	HD11) HG21)	HD24)	KB1	HO24)	HD 1)	HG2))	HG1))
and name and name ak 26092	11d 110 and name 11d 116 and name 1.800 peak 26122	aid 110 and name aid 116 and name 2.200 peak 26132	oid 110 and name id 113 and name 1.400 peak 26142	sid 116 and name sid 117 and name 1.300 pesk 26213	resid 116 and name resid 79 and name 2.300 peak 26222	and 116 and name aid 115 and name 1,700 pask 26242	resid 116 and name resid 116 and name 1.800 peak 26252	resid 116 and name resid 110 and name 2.100 peak 26262	reeld 116 and name reeld 107 and name 2.100 peak 26122	and name and name ak 26372	and name and name ak 26382	and name and name ak 26402	and name and name ak 26412	and name and name ak 26432	aid 116 and name HD14) aid 76 and name HD24) 0.600 peak 26472 weight	sid 116 and name and 110 and name 1.000 peak 26482	sid 63 and name HD2%) sid 60 and name HA)) 1.300 peak 26502 weight	resid 116 and name resid 115 and name 1.100 peak 16522	11d 116 and name 11d 110 and name 1.900 peak 26532	sid 116 and name sid 110 and name 2.200 pesk 26542	aid 103 and name aid 104 and name 2.200 peak 24682	id 94 and name HUI)) id 91 and name HBI)} 0.100 peak 26692 weight
1110 1110 100 Pe	d 110	d 116	resid 110 resid 113	resid 116 resid 117	300	resid 116 resid 115 1.700 pe	4116 1106	911 P	d 116	4 75 1,300 pe	d 116	d 116	d 116	14 78 Pe	resid 116 resid 76 0.600 pe	resid 116 resid 110 1.000 pe	resid 63 resid 60 1.300 pe	14 116 11.100 pe	resid 116 resid 110 1.800 pe	resid 116 resid 110 2.200 pe	resid 103 resid 104 2.200 pe	resid 94 resid 93 resid 94
and resi	and rear	::	2 2	2 2	and rees	öö		3 3	and ree	and resi	and res	and resi	and resi	and rea	2 2	5 5	2 2		2 2	4 6		
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ASSI (2692) [eegid 'STD' and resid 110 and name [eegid 'STD' and resid 111 and name [eegid 'STO' and resid 111 and name	f megid "BrD" and resid 110 (megid "BrD" and resid 11s 1.00	(segid SEC and resid 110 and (segid SEC and resid 116 and 11	2.400		(segid BrD and (3.200 2.600	(segid 'BrD ' and r ((segid 'BrD ' and r).600 3.600	(aegid 'B (2.700	2.400	(megid "BYD " and r. (megid "BYD " and r. 3,200 2.600 AGBI (26372)	3.200 1.200 2.200	3.400	1 2640 (megid (megid 2.600	(megid (megid 2.100	Absi (4642) (1642)	(eegid BrD and (eegid BrD and 4.900	(segid 'BrD ' and (segid 'BrD ' and 2.000	(eegid 'Brb ' and (eegid 'Brb ' and 2.300 2.300	((megid "B ((megid "B (, 400	([segid BrD snd [segid BrD snd [segid BrD snd].600	(eegid "BrD " and r. (seegid "BrD " and r. 3,300 2,700	(megid 'Bi	(eegid BrD and (eegid BrD s.400 S.400 S.400 (eegid BrD and f.400 S.400 (eegid BrD and f.400
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5.642 ppm2

3.117

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1.401

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4.4

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3.02

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5.843

2.930 ppez 2.733 ppm2

2.00

2.781 ppm2

5.5

1.

2.815 ppm3

1.572

3.421 ppm3

4.265

3.423 ppm2

2.454

3.423 pom2

1.36

3.962 ppm2

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3.912 ppm2 3.902 ppm2

3.

1.079

2.339 ppm2

1.075

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4.972

4.163 ppm2

5.539

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2.30

3.423 ppm2

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KD24) KE4)	MD24)	KDIVI C	Might HD10)	MD14)	KB1)	HD24)	HB1.)		4619ht HD14) HD24)	HD1V)	MD2V)	HD21)	We 19ht HD24) HZ 1)	HD24)	HD2N) HA))	HD2N) HA 1)	HD24)	HD24) HB))	MB1))	MB2)) MG1))	HB1	100	MB2))	() H
11			: II	062	100	Dame H				D 202			Dame H	223	112		# # 55 # # 55	Dame H	115					
9 9	and name	99	and new	A 20	peak 20102	9 9 4	and name and name	22	and nems		and name	and name		and name and name peak 20292	and name and name peak 28322	and name and name pask 28343	and name and name peak 20152	and name and name	and hame and name peak 28402	and name and name peak 20412	2 2 2	99	and has	2 and name and name peak 28532
2.2	2 2 2		2.000 p	2.000 p	0.800 p	11d 78 and name 11d 106 and name 3.100 peak 28122	resid 16		. pi	, pi	26 bid 36	3 7 7	A	2.000 P	\$ 7 2		atd 78 1.700 P	_	3 2 5	1. 50 P	resid 102 and name resid 62 and name 2.100 mesk 28442	sid 102 and name	id 103	3 2 8
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9.0	66	29	200	2		20	9.00		9.0	- e c	28262) egid BrD	<u>.</u>	2.5	20		eegid BrD			91d BrD 91d BrD		istt2) gid 'BrD gid 'BrD	4 6 E	- C. C.	
megic 2003		ASSI (28032) (megid "B ((megid "B	~~ = =		• • -		(76112) eegid 'B	I (28192) segid 'BrD " and re (segid 'BrD " and re	ASSI {28202} [eegid BrD end { eegid BrD end				OR (28272) (segid ((segid	ABSI (28292) (amgid "BrD " and r ((amgid "BrD " and r) 3.00 3.100	9 10 10 10 10 10 10 10 10 10 10 10 10 10	900.0	segid BrD and re (segid BrD and ra 3.600 3.600	- 6 6 4 -	91d 91d 1.800	- 4 4 +	- 4 4 0	ASSI (28472) ((eegid 'BrD ' end : (segid 'BrD ' end :), 200 2 600	ASSI (18502) ((amgid 'BrD - and r (megid 'BrD - and r) 600 1.200	((eegid (eegig) (ee
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0.549548+02	0.373538	301160		0.540528	. 5663	.5407	0.806818+02	0.624388	0.3107016-03	.860528+02	0.176868	0.10158K+04	0.111378-03	. 550688900	0.262856+02	119	0.172218+02	0.222746+01	0.100778+03		0.34865E+02	.34614	.7639.	0.634176.03
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o						0.10	0.10										9.10				0.10	0.10	0.10	0.10
KA 1	HOIS)	KD24) HG14)	H 602	HD24)	weight	HE'S	KD14) HB1))	HD14) HEA)	KD14)	HB14) HB2 1)	HD24) HB%)	KA)) KB2)) Veight	HA)) HG16) weight	HB2))	HB1))	HB2)) HO11)}	HB2);	HO))	HO)) H2))	HG)	NB2)) KD%) weight	HEL)	HD24) HD4) Weight	HD24) HZ)) weight
1392	7442			and base	7492	and name	and name 1 and name 1 ak 27572	7582	7632	7662	name name 7692	7712	name 	0.00mm 0.00mm 1777	7822	7843	and name t and name t	7002	Dame 1			Dame H		7992
and name peak 27392	and name and name peak 27442	and name and name peak 27452	and name and name		y S		334	and name and name peak 27582	and name and name peak 27632	and name and name peak 27662	and name and name pask 27692	and name and name peak 27712	and name and name peak 27722	and name t and name t peak 27772	and name and name peak 27822	and name and name peak 27842	and name and name peak 27872	and name and name peak 27882	and name and name peak 27892	9 5	and name and name peak 27912	and name to and name peak 27942	and name and name wak 27982	and name and name peak 27992
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d reald	d regid	resid	d resid			2.	d resid	d resid	200	d resid	d reald d reald	d resid	d resid		d resid	d resid	d resid	d resid	d resid	P	d reald	Past Past Past Past Past Past Past Past	resid	d resid
2.968		9 4 9	4 4 6	4 4	1.300	2.5	2.6 6 \$ 8	1.200	1.600	2.400	2.000	1,100	2.200	2.900		4 4 6	100	5.500	2.500	• • •	3.200	700	1. 200	D - and re
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- 11	;	2	ASS.	ASE)	ASS	Y T			7			===	3 - C	7 T	18 T	===	3.5	3 .	1 5	= = =	- 1			5

0.662 ppm2

0.10000E+01 volume 0.14234E+03 ppm1

4.727

0.761 ppm2

0.43609E+02 ppm

0.10000£+01 volume

0.10000E-01 volume

4.525

0.761 ppm3

3.910

0.763 ppm2

0.775016+01 ppm

0.10000E-01 volume

1.703

0.662 ppm2

3.919

0.662 ppm2

0.122766.03 ppm

0.10000E+01 volume

0.10000E+01 volume

0.10000E.01 volume

2.063

0,760 ppm2

1.590

0.761 ppm2

0.29008E+03 ppm]

0.10000E+01 volume

0.424 7.534

0.760 ppm2

0.64808E.02 ppm

0.10000E+01 volume 0.10000£.01 volume

1.254 ppm2

0.17777E+02 ppm1

7.041

1.253 ppm2

0.54803E+02 ppm1

volume

5.371

1.254 ppm2

0.41030E+62 ppm

0.10000E-01 volume

4.509

1.254 ppm2

4.733

1.251 ppe2

0.99&05E+02 ppm

0.10000E-01 volume

0.10000E+01 volume

3.95

1.254 ppm2

.00

1.254 ppm

0.41722E-02 ppm1

volume

3.451

2.684 ppm2

0.28628E+02 ppm1

3.45

1.993 ppm2

0.20241E+02 ppm1 0.137086.03 ppm1

volume

0.10000E.01

7.064

1.993 ppm2

T. T.

. 842 ppm2 1.842 ppm2

0.70904E+02 ppm1

volume

99. .0 7.041

0.34445E+02 ppm1

3.141 ppm3

0.25286E+03 ppm1

VO) take

A881 (29052)	ASSI (2912) (eegid BED ((eegid BED (3.600 ASSI (29142) (eegid "BrD " ((segid "BrD "	4.500 4.1 ABSI (29172) (segid BED •	3.500 3.1 ASSI (29222) [segid BrD * (secid BrD *	2.600 2.0 A881 (29212) { eegid BrD •	2.900 2.3 OR (29212) (segid BrD (ASSI (29392) (1 eegid "BrD" (segid "BrD" 3.300 3.6	ABB1 (29302) (eegid BrD • (eegid BrD • 3.000 2.2	AGSI (29362) (eegid BrD (eegid BrD)	ASSI (29472) ((eegid *BrD * ((eegid *BrD * 3.700 3.4	OR (29472) ((megid "BrD = ((megid "BrD = ABB! (29602)	(eegid 'BrD ' (eegid 'BrD ' 3.600 3.2	((segid BrD * (segid BrD * 3.4	((segid 'BrD ' ((segid 'BrD ''	(eegid '9rD ' (eegid '9rD ' (eegid 'BrD '		ABSI (29662) ((eegid 'BrD ' ((eegid 'BrD '),100 2.4	- 5 5	_ = = =	A581 {29752} ((aegid '8rD '	22	(29782) eegid 'Br eegid 'Br	AESI (29792) ((segid "Brī ((segid "Brī
	7.534	5.553	4.525	4,354	5.574	3.82	2.473	0.676	1.750	5.395	£.413	4.436	0			i i			1.263	1.451	4.900		
1.303 poes			1.303 ppm2	1.303 ppm2	bbw3	Ç d				2.141 ppm2 s.	ppm3 .			<u> </u>				2.148 ppm2					
.10000E+01 volume 0.38923E+02 ppm1	e 0.8642E+02 ppm1	- 0.836008+02 ppm1	e 0.15974E+03 ppm1	e 0.447508+02 ppm1	0.73306E+02	0.362898+03	e 0.68536R+02 ppm1	0.555548.02	e 0.67664E+03 ppm1	e 0.10599&+03 ppm1	0.459325.03	e 0.181235+03 ppm1	0.476045.03	0.194678+02	0.263328.03	0.697068.03		. 0.19745E+02 premi		0.338498+02	0.163198+03	. 0.32346E+03 ppm1	0.223448.04
۰	۰	 		 	 } E 0.10000E+01 volume		1) 1t 0.10000E+01 volume	A 0.10000E+01 VOLUME	1 0.10000E+01 Volume))))))))))	.)))))) .) nt 0.10000£+01 volume	1) 10 0.10000E+01 volume	0.100006+01		0,100005+01)) it 0.10000E+01 volume) R 0.10000E+01 volume) r 0.10000E+01 volume) ic 0.100008+01 volume) it 0.100005.01 volume
(segid "BrD * and resid 102 and name HD2t) (segid "BrD * and resid 62 and name HDt) 3.600 1.200 1.900 peak 28562 weight			[eegid BFD * and resid 102 and name ND24] (eegid BFD * and resid 106 and name HA)] 2.800 2.000 peak 28632 weight and facts!	[eegid BrD	Acas (asses) (a segid 'BED' and resid 102 and name HD1%) ((segid 'BED' and resid 28 and name HD2)) 1,000 2.600 2.300 peak 28662 weight	4 eegid '9FD' and resid 102 and hame HD24) (4 eegid '9FD' and resid 105 and name HB1)) 3.600 1.300 1.300 peak 28702 weight and fearal			decid BED and resid 115 and name HD1t) (segid BED and resid 17 and mame HG2t) (segid BED and resid 17 and mame HG2t) are 12.200 1.200 peak 28782 weight	((segid 'BrD ' end resid 66 and name HG2)) ((segid 'BrD ' and resid 65 and name HA)) 3.000 2.300 2.200 peak 29792 weight	(6 megid "BrD" and resid 115 and name HB1)) (6 megid "BrD" and resid 110 and name HA)) 2.00 1.400 1.400 pask 28812 weight	(aegid "BTD" and reaid 115 and name HG)) ((segid "BTD" and reaid 110 and name HA)) 2.800 2.000 peak 28822 weight	(eegid and resid 115 and name HG)) (eegid BED and resid 110 and name HD18) 1.400 2.100 peak 28842 weight	AESI (28852) ((segid "EED " and resid ll5 and name HB1)) (segid "EED " and resid ll3 and name HBN) 1.600 1.200 1.900 peak 28852 weight	[26872] segid 'BID' and resid 115 and name segid 'BID' and resid 110 and name 2.600 2.600 1.900 pask 28872	2002] egid 'BrD' and resid 115 and name egid 'BrD' and resid 116 and name 7200 1.200 peek 2862	(6 segid 'BrD ' and resid 115 and name (B1)) (6 segid 'BrD ' and resid 115 and name (G2))		(28812) (28812) 2021 deld "BED" and resid 115 and name 8651d "BED" and resid 110 and name 3.400 2.900 2.100 peak 28912	resid 56 and name resid 35 and name 1.900 peak 28932	Ames (18952) (segid 'BrD' and resid 56 and name MD18) (segid 'BrD' and resid 35 and name NA.)) 2.800 2.000 pask 28942 weight		139042 1

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1.083

1.947 ppm2

0.403218+02 ppm1

1.86

2.535 ppm2

0.105586+03 ppm1

7. 111

4.361 ppm2

0.67859E-02 ppm1

5.018

2.779 ppm2

0.322108+02 ppm1

2.443

4.360 ppm2 4.755 ppm2

0.85748E+02 ppm1

volume

4.550

\$.000 ppm2

volume

D. 10000E+01

5.000 ppm2

volume

0.10000E+01

5.003 ppm2

4.755 ppm2

0.51818E-01 ppm1

0.10000E+01 volume

1.90\$

4.804 ppm2 5.445 ppm2

0.13311E+02 ppm1

0.10000E+01 volume

0.10000E+01 volume

0.10000E-01 volume

0.030

4. 808 ppm2

1.604

4.507 ppm3

0.72004E+02 ppm1

4.607 ppm3

0.52302R+02 ppm1

0.10000E+01 volume

2.45

5.346 ppm2

0.10000E+01 volume 0.37115E+02 ppml

| 1.00 peak 2013 | 1.00 peak 10.00 | 1.00 peak 2013 | 1.0

sand of the sand o

4.516

0.98620E+01 ppml

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2.536 ppm2

0.405578+02 ppm1

volume

2.881

2.536 ppm2 2.535 ppm2

0.17311E+03 ppm1

volume

3.19

0.12717E+03 ppm1

1.966

1.847 ppm2 1.847 ppm2

0.36305E+02 ppm]

volume

3.003

1.848 ppm2

0.33714E-02 ppm1

0.10000E+01

	resid 19 and name resid 15 and name	3.200 2.600 2.300 (10962) megid Bib and resid Si	augus oru end resid St. and hame (31062) eegid 'BrD' and resid 22 and name	eegid "BrD " and resid 74 2.500 2.500 2.000 (31162) aegid "BrD " and resid \$4	### 2 #### 2 ### 2 ### 2 #### 2 #### 2 ##### 2 #### 2 #### 2 #### 2 ######	2.900 2.100 2.100 peak [2.3] eegid BrD and resid 47 and seegid BrD and resid 47 and	2.300 peak 23	3.600 3.600 1.700 peak 43 (5.5) egid 'BrD' and reeid 46 and name	4.000 4.000 1.500 peak 5) [93] 4.000 1.500 peak 5)	aegid BrD and resid 46 and name 2,600 1,700 1,700 pask 91	segid BrD and resid 46 and name segid BrD and resid 88 and name 1.100 1.100 peak 101 { 111}	(segid "BPD and resid 46 and name MEV) ((segid "BPD and resid 46 and name MEN)).300 and 2.700 peak 113 weight	113} emgid 'BrD * and resid 46 and name emgid 'BrD * and resid 46 and name	(153) (153) (153) (153) (153) (153) (153) (153) (154) (and Dame	segid '8rD' and resid 26 and name 3.600 3.200 1.900 peak 273 8.013 9.010 and resid 67 and need	2.200 peak 333	Megan BrD and resid 67 and hame gold BrD and resid 68 and hame 2.000 2.000 2.000 peak 343 { 353}	eegid BrD and reald 67 and name eegid BrD and reald 67 and name 2.500 1.600 1.600 peak 353 { 373}	megid "BED" and resid 67 and name segid "BED" and resid 67 and name 3.300 1.300 1.300 peak 373 (383)	degid 'BFD' and resid 67 and name segid 'BFD' and resid 68 and name 3.900 7.100 7.100 pask 383 ft 603 ft 603 ft 603 ft 600 ft 60	reaid 68 and 1.400 peak	(could be properly and resid as and man (ks.) (could be properly and man (ks.) (could be properly and could	2.100 2.100 peak 463
	5.390	5.390	7.488	7.488	5.367	\$. 29 \$	1.550	1.551	4.011	,		7.691	7. 815	1.489	7.722	3.028	2 204			4. 50 to 10		1.508	2.964	
	3.631 ppm2	3.673 ppm2	1.671 ppm2	3.631 ppm2	5.001 ppm2	3.614 ppm2	2.413 ppm2	1.701 ppm2	4.459 ppm2			1.946 ppm2	1.946 ppm2	2.190 ppm2	1.891 ppm2	0.760 ppm2	1.692 pms			3.029 ppm2	1.994 ppm2	4.656 ppm2	4.653 ppm2	٠
	0.190676+02 ppm1	0.127378+02 ppm1	0.17551E+03 pp=1	0.20\$20E+03 ppm1	0.40427£+02 ppm1	0.75028R+01 ppm1	0.214316+02 ppm1	0.22947E+02 ppm1	0.72129E-01 ppm1 .	91298R+02		0.12241E+03 ppm1	0.96863E+02 ppm1	0.45416K+03 ppm1	0.305018+02 ppm1	0.52723K+02 ppml	0.497678+03 ppm1.			0.255938.02 prest		.34166E+02 ppm1	0.26014E+02 ppm1	
	.10000£+01 volume 0	.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01. volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000E+01 volume 0.		10	0.10000E+01 volume 0	0.10000E+01 volume 0	0.10000K+01 volume 0	0.10000E+01 volume 0	0.10000E+01 Volume 0	e milos	1		vo) ume	.10005E-01 volume 0.	0.10000E+01 volume 0	
and name HB1)) and name HB2)) and name HB2))	and name and all	and name HA)) peak 29842 weight 0	and name HD1)) and name HE%) pmak 29852 weight 0	HEA)	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	45))	(1016)	(014) (014)	and name MA)) and name MD2)) peak 10022 weight 0	HB2)} KB1)}	and name HG11)) and name HG11)	H011)	weight HG1))	D24)	oi) oight	and name HG2)) and name HG1)) peak 30322 weight o	and name HB2 }) and name HBb } tak 30362 weight.	El)	KEZ)	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	HD1)) HO1))	eid 109 and name HA)} sid 21 and name HG2b) 1.900 peak 30682 weight 0	aid 109 and name HA) aid 112 and name HG1) 1.700 peak 10702 weight 0 sid 109 and name HA)	name HG2
2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	1. Soc	1.200	2.000 2.000	maid 66 mead 15 1.800	7001d 65 7000 2.000	914 'BrD' and resid as 914 'BrD' and resid 65 992} 914 'BrD' and resid 66	1.600	1.600	0.000	id BrD and resid 103 and name id BrD and resid 82 and name 100 2.400 2.400 peak 30062		2 2	2.400	3.100 2.000 p	91d "BFO " and resid S6 and neme H 91d "BFO " and resid 96 and name H 700 3,400 1.800 peak 30262 w	resid as 2.100	4.5	2 2	esid 10					Piess
OR (19792) ({ eegid "BrD" and r ({ eegid "BrD" and r (f eegid "BrD" and r	4.000 ABSI (29642) ((segid "BED				2 2	((aegid 'BrD 4.700 A881 (2992) ((aegid 'BrD		• •			2 4 5 2	211	3.100 ASSI (10162) ((megid "BrD	2 42	8845		angid Br		ABSI (10492) ((megid 'BrD " end r ((megid 'BrD " and r 3.000 3.200	ABS1 (30502) ({ segid "BrD " and 1 ({ segid "BrD " and 2 3.600 3.600		200 Br	3.00 to 1.00 t	P Bee

3 ...

.486

2.289 ppm2

0.10000E+01 valume 0.75523E+02 ppml

0.10000£+01 volume 0.81070£+02 ppml

0.10000E+01 volume 0.51425E+03 ppml

7.497

1.388 ppm2

3.288 ppm2

0.100005+01 volume 0.89147E+02 ppml

5.754 ppm2

0.11000E+01 volume 0.62066E+02 ppm1

7.421

6.688 ppm2

0.11000E+01 volume 0.11086E+02 ppm1

5.758 ppm2

0.11000E+01 volume 0.31210E+02 ppm1

1.154

5.758 ppm2

0.11000E+01 volume 0.11748E+03 ppml

0.11000E+81 volume 0.78634E+81 ppm

. 688 ppm2

0.11000E+01 volume 0.25301E+03 ppm1

6.129 ppm3

0.110008-01 volume 0.14248E-02 ppml

0.11000E+01 volume 0.41792E+02 ppm1

0.11000E+01 volume 0.67483E+02 ppm

5.758 ppm2

0.11000E+01 volume 0.14809E+03 ppml

. 685 ppm2

0.11000E+01 volume 0.42674E+03 ppm1

.67

. 246

. 474 ppm2

0.11000E+01 volume 0.22980E+03 ppm1

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4.711	£. 69 .	5.452	3.942	4.373	4.62	3.618	3.6	1.63	3.643	6.938	•	5.146	3.673	6.693	5.745	4.999	4.939	4.154	1.511	1.431	1.3%	4.965	
7.246 ppm2	7.942 ppm2	8.455 ppm2	. 456 ppm2	7.013 ppm2	7.664 ppm2	7.664 ppm2	7.666 ppm2	Zudd	bba2	ppm2	bbws	Z model	ppe 3	pp.	čedk č	ppm2	ppu-	ppe 7	ppm2	bbwg	Ppm2	. 74	1
7.246	7.942	6.455	4.456	7.013	7.664	7.664	3.6	7.474 ppm2	7.478 ppm2	7.850 ppm2	7.850 ppm2	7.850	7.757 ppm2	7.618 ppm2	7.616 ppm2	7.616 ppm2	7.410 ppm2	7.618	7.616 ppm2	7.711 ppm2	7.712 ppm2	. 2.708 ppm2	
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7001E+02	0.296228+03	0.104498+03	0.53265E+02	0.154708+03	0.617356.03	0.19360£+03	0.489358+03	0.179076+02	0.775156.01	0.398086+02	0.57511E+02	0.51154E+02	597368+03	0.627648+02	0.387366+02	0.31179E+03	D.64049E+02	0.385622+02	0.210106+03	8299E-03	0.196878+03 ppml	0.26381E+03 ppm1	
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volum	volume	vol une	volume	volume	volume	emu lov	volume	volum	vol une	volume	volume	volum	vol ume	volume	vol una	vo) ume	vol une	volume	volume	volume	volume	volume	
0.11000E+01 volume 0.27001E+02 ppms1	0.11000E+01	0.11000£+01	0.110005+01	0.11000E+01	0.110002+01	0.110006+01	0.110008+01	0.11000E+01 volume	0.11000E+01 voluma	0.11000E+01	0.11060E+61 volume	0.11000E.01 volume	0.11000E+01	0.11000E+01	0.11000E+01 volume	0.11090E+01 volume	0.110006+01	0.110008+01	0.11000E-01 volume	0.110006+01	0.110008+01	0.11000E+01 volume	
																							_
HEA)	KD()	161)	HB1))	HDA)	HD.	HB1))	HDA)	HEN)	HEN) HBZ))	HD&)	HEA)	KG.)	KDA) KB1))	HE'S I	KDV)	HDA)	HE)	NO.	HDI)	HDA)	KB1)	HOL.	H H H H H H H H H H H H H H H H H H H
and Do	d heme	and name and name ak S43	d Dame	d name of name	4 de la compa	d hame	d name d name	d Pame est	d Deme	d name d name	d name d name 1003	4 neme	d name 1213	d name d name 1263	d name 1283	4 name	d name Litt	P 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	2 mm	d name d name 1403	A 0.051	d name d name 1503	2 2
Pash day	7 2 2	X.	2 and a	b and	Para Para Para Para Para Para Para Para	* 5 5	2 4 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5	2 2 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	P P P P	and and	Pethod	P P P P	P P P	A P	Pe and w	pask k	De a sad	F & & &	2 5 4 5 E	Pa and	1 2 4	P & S &	5 C
raeid 47 raeid 47 2.200	resid 47 and n resid 47 and n 1.200 peak	resid 32 resid 30	resid 32 2.100	resid 74 resid 74 1.600	resid 15 resid 15 0.900	resid 15 resid 15 1.400	resid 15 resid 15	resid 15 resid 15 2.000	reald 15 reald 15 1.500	resid 68 resid 74 2.400	resid 68 resid 67 2.100	resid 68 2.100	resid 68	resid BB resid 46 2.000	Feeld 88 Feeld 46 2.400	resid as resid as	resid 88 2.000	resid 88 2.400	reeld 88 reeld 88	resid 96 resid 96 1.400	reald 96 1.400	reeld 34 reeld 31 1.200	resid 107
6 6 5	0 * *nd	0 * and 1.700	2.100	1.600	P 0 0	3 5 9	. 000 t	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	9 0 0 0 0 0 0	9 9	2.100	2.100	Pu 000	pu	9 0 0	9 9 9	pu • 000	9 9 9	D . and 1.300	and 1	Pu o	1.200	9 9
22.	ee"	22	99	22	Q Q	original and a second	22	22	2 .	9.0	99	0.0	ou i	ord ord	9.0	22	22	0.0	22	e de	e e	20	segid 'SrD' and :
megid "BrD " and a segid "BrD " and a 3,700 2,700 [503]	segid BrD and r 2.200 1.200	segid BrD and segid BrD and 2.600 1.700	eegid BrD and seed are and are	segid BYD and a	segid BrD and	segid "BrD " and r. segid "BrD " and r. 2.400 1.400	megid BrD and megid BrD and 2.000 1.000	megid BrD and 1 1-500 3.100	aegid 'BrD ' and r. (aegid 'BrD ' and r. (.000 (4.000	eegid 'BrD and and 1.100 2.400	segid "BrD snd r segid "BrD snd r 2.900 2.100	megid BrD and megid BrD and 2.900 2.100	segid "BID" and r segid "BID" and r 2.000 1.000	segid BrD and a segid BrD and 2.000 2.000 [1283]	eegid BrD and r eegid BrD and r 3.100 2.400	aegid "BrD " and r aegid "BrD " and r 2.200 1.200	##91d BrD and r #91d BrD and r 2.800 2.000	megid 'BrD ' and segid 'BrD ' and s 3.100 2.400	segid BrD and segid BrD and 2.300 1.300	segid 'BrD and 1 segid 'BrD and 1 2.400 1.400	segid BrD and segid BrD and 1.400	segid 'BrD' and a segid 'BrD' and a 2.200 1.200	916e
A681		==	== ;	j-= j	-=	j-=	-=	-= 1	1		8) F	i	7 7 7	- 5	- 3 ig	, , , , , , , , , , , , , , , , , , ,		- 5	- 3	-=] - E

	727							7.261	1.076	1	6	1.520	6.823				1.1	1.336		1.837	3.654		3.933	100	
1333 1400	7.686 mm2		7.47	7.617 ppes	7.619 pond	7,614 8922	1,77	7.013 ppm3	6.688 ppm2	5.750 0000	6.130 pos	6.129 ppm2	6.129 pom2	7.524 800.2	2.060		7.757 ppm2			7.413 ppm2	7.711 ppm2		7.603 ppm2	7.603 ppm2	:
11.00	0.29123E+02 pum1	0.22641E.02 DDm1	0.35285K+03 ppm1	0.235916-02 ppm1					0.48608K+02 ppm1	0.36832E-02 ppm1	0.66486R+03 ppm1			0.13584E+02 ppm1			ä			1.21121E-02 ppm1	.40018K+02 ppm1			.30863E+02 ppm1	
### 1719 2.00	0.11000E-01 volume	volume	volum	3.11000E+01 volume	volume	volume	volve	volume	volume	volume	.10000E+01 volume (volume	volume		volume	vol ter	votume	volume		.10000E-01 volume 0	volume		volume	.10000K+01 volume 0	
1110) 1100 1110) 1110 1110 1110 1110 11	1543	name HD4) name HB2)) 1793 weight	name MDV) name MA)) 1833 veight	name HEV) name HA)) 1883 waight	name HEt name HHZ) 1943 weight	name KEA) name KZ2)) 1943 weight	name HH2)) name HZ2)) 2023 weight	name HZ)) name HDN) 2133 weight	name HEN) name HOIN) 163 weight	name HDA) name HB ()) 163 weight	name HEL !) name HG24! 253 weight	name HE1)) name HD10) 263 weight	Dame KE1)) Dame H91)) 20) weight	name KEt) name HD14) 733 weight	name MD4) name MD4) 793 weight	name KD1) name KD2)) 1113 weight	name MD1 } name MB2 } 1113 weight	Dame 1173	11		name ND4) name NB1)) 1423 weight	name MDA	name KD4) name KB1)) 1613 weight	I name KDt) I name HA)) 1663 weight	d name HEb)
(130) 1.00	2.300	reald 95 reald 95	resid 95 resid 95	reeld 95 2.100	resid 95 resid 32 0.800	resid 95 resid 32 2.100	resid 32 Feeld 32 1.100	reeld 82 reeld 82 1.700	reeld 46 reeld 38 2.200	resid 46 resid 50 2.400	reald 28 7.000	resid 28 1.700	reeid 28 2.100	::	reeld 82 Fasid 100	reeld 68 1.700	22	d resid 105 and resid 105 and 2.000 peak	2 2			eaid 100	::	reeld 107 reeld 103 2.400 pe	106
	3.200	1.400				2.400 d										2.600 2.600 2.600	9 9 6			(eegid 'BrD " an (eegid 'BrD " an 3.400 2.900 11 (1423)	(megid 'BrD ' an (megid 'BrD ' an 1.100 2.400	(aegid 'BrD - and (aegid 'BrD - and it 1613)	aegid BrD - aegid BrD - 3.600 3.5	segid BrD	(segid 'BrD ' and

3.708	3.571	7.076	3.007	6.613	3.304	4.586	3.780	4.430	1.706	1.545	4.	2.781	2.211	3.803	4.439	7.927	7.793	2.3	3.154	7.787	-0.311	2.667	
7.265 ppm2	7.262 ppm2	7.263 ppes	7.005 ppm2	5.743 ppm2	5.740 ppm2	5.57 Ppe	7.265 ppm2	6.63 ppas	6.489 ppm2	6.839 ppm2	4.490 ppm	8.490 ppm2	6.490 ppm2	6.008 ppm2	8.058 ppm2	8.058 ppm2	8.058 ppm2	8.059 ppm2	6.008 ppm2	8.004 ppm3	7.959 ppm2	7.961 ppm2	:
0.67788£+03 ppm1	0.77298£+03 ppm1	0.12642E+04 ppml	0.64123E+03 ppm1	0.17599E+04 ppm1	0.61947E-03 ppm1	0.15484E-03 ppm1	0.224326.03 ppm1	0.89209K+02 ppm1	0.21286E+01 ppm1	0.64742E-02 ppm1	0.97341E+02 ppm1	3880K-03 ppm3	0.301176+02 ppm1	0.142398+03 ppm1	0.17934E-03 ppm1	0.19563R-04 ppml	0.49678E+03 ppm1	0.34018E-03 ppm1	1123£-03 ppm1	0.13157E+04 ppm1	0.11962E+03 ppm1	0.29398E+03 ppm1	
* 0.10000E.01 volume 0.6	volume	volume	volume	volume	volume	vol in	volume	vol ume	volume	volume	volume	01 volume 0.16	volume	volume	volume	volume	volume	volume	01 volume 0.45	-01 volume 0.13	0.10000E+01 volume 0.11	0.10000E+01 volume 0.29	
	1) 16 0.10000E+01	nt 0.10000£+01	1) 10 0.10000£-01	1E 0.100005+01	1) 10 0.100002-01	1) 14 0.10000E+01	1) 14 0.10000E-01	1) 10 0.10000E+01))))))	1 0.10000E+01	1) 10.10000E+01	1) 15 0.100008+01	1) 10 10 10 10 10 10 10 10 10 10 10 10 10	1) 1) 1c 0.10000£.01	1) 3c 0.100008+01	1) 1c 0.100008+01	1) NE 0.10000K.01))))))))))) it 0.100008+01)) ie 0.10000E•			
name HDt) name HB1 !) 3204 weight	neme ND4) neme NB2)) 1214 weight	name HDt) name HBt) 3304 weight	name HDt) name HB2)) 3644 weight	name MDt) name MEt) 3694 weight	neme HD1) neme HB1)) 3914 weight	name MD2 1) name MA 1) 4064 weight	name KDV) name KA)) 64 weight	neme HD4) hame HA 1) 174 weight	name HD4) name HB2)) 244 weight	name KD1) name KD11) 254 weight	neme KD1)) neme KA)) 464 weight	name HD1)) name HD1)) 494 weight	name KD1)) name KD2 }) \$04 weight	name HZ)) name HB1)) \$64 veight	name KZ 1) name KA 1) 624 weight	name HE 11 name HEN 1 634 weight	name NZ 1) name NDt 1 644 weight	name HZ)) name HOL)) 664 weight	name H22)) name H01)) 694 weight	neme HZ2)) neme HZ3)) 714 weight	name KE3) name HG2 } 724 weight	neme HZZ }) neme HB1) 804 weight	
said 82 and 1.400 peak	resid 82 and resid 82 and 1.300 peak	reeld 82 and reeld 82 and 1.100 peak	resid 74 and resid 74 and 1.400 peak	resid 46 and 1 resid 46 and 1.000 pesk	resid 46 and resid 46 and 1.400 peak	resid 28 and resid 2 and 2.200 peak	resid 82 and resid 103 and r	resid 67 and resid 62 and 2.200 pesk	id 67 and id 62 and 7.100 peak	resid 67 and resid 73 and 2.000 peak	resid 12 and 1 resid 29 and 1 2.200 peak	reald 32 and 1 reald 33 and 0	resid 32 and 1 1.500 peak	reeld 107 and I reeld 79 and I	resid 107 and r resid 79 and r 2.200 peak	resid 107 and r resid 107 and r 1.000 peak	resid 107 .and r resid 107 and r 2.000 peak	aid 107 and aid 79 and 1.800 peak	resid 32 and a resid 94 and a 1.600 peak	resid 32 and r resid 32 and r 2.400 peak	resid 32 and resid 33 and 2.300 peak	resid 12 and resid 97 and 1.800 peak	reeld 32 and reeld 32 and
2.2	1.300	0 • end reeld 0 • end reeld 1.100 1.3	22	. and res	3 . and res	2.200	2.100	2.700 ' .	2.100	3.100	2.700	5.500 (4.000	2.400	2.200	• •	2.500	1.800	and resi	2.100	2.600	and resi	and read
	aegid 'BrD and : 2.300 1.300	egid arD and regid arD 2.100 1.100	aegid BrD and 2.400 1.400	aegid 'BrD and r. aegid 'BrD and r. 2.000 1.000	aegid "BrD and r aegid "BrD and r 2.400 3.400	(segid '8tb ' and r (segid '8tb ' and r 3.000 2.200	aegid 'BrD ' and r aegid 'BrD ' and r 2,900 2,100	aegid 'BrD ' and 3.300 2.700 (244)	egid "BrD " and resid 67 and na (segid "BrD " and resid 62 and na 2.90 2.100 2.100 peak 7 [254]	eegid arp and r eegid BrD and r 3.500 3.100	megid 'BrD ' and re 3.300 2.700	eegid 'BrD and eegid 'BrD and 5.500 \$.500	(aegid *8rD * and r (aegid *8rD * and r 4.000 *.000	eegid 'BrD ' and eegid 'BrD ' end 3.100 2.400	eegid 'BrD ' and r eegid 'BrD ' and r 1.000 2.200	magid 'BrD and r. aegid 'BrD and r. 2.000 1.000	eegid BrD and z eegid BrD and z 2.500 2.500	{ eegid 'BrD " end resid 107 e { eegid 'BrD " end resid 79 e 2.700 1.800 h.800 pee 1. { 694}	aegid BrD and r aegid BrD and r 2.500 1.600	eegid BrD and 2.100 2.100	eegid BrD and a eegid BrD and a 3.200 2.600	(segid 'BrD ' and r. (segid 'BrD ' and r. 2.700 1.600	(86gid 'BrD ' and i
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š	5	\$ 30		143	• 0	6 09	040	90	5	121	•	140	996	•	7.1.	313	11¢	•	124	115	3	100	•

7.778 ppm2

0.56412E+03 ppm1

0.10000E+01 volume

| 1.100 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.400 | 1.40

AND THE PROPERTY OF THE PROPER

7.718 ppm2

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0.81340E+03

0.10000E+01 volume

7.612 ppm2

M

0.10000E+01 volume

6.491 ppm2

Mdd

0.10000E+01 volume

1.490 ppm2

0.14234E+03 ppml

0.10000E+01 volume

7.781 ppm2

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0.10000E+01 volume

MEN) MB1)) weight

1.724 ppm2

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0.297445.04

0.10000E+01 volume

7.726 ppa2

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6.899 ppm2

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0.10000E+01 volume

7.617 ppm2

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0.10000E+01 volume

1.478 ppez

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volume

7.479 ppm2

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1.478 ppm2

PP.

0.100008+01 volume

7.618 ppm2

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volume

7.757 ppm2 7.013 ppm2

E E

0.521926+01

0.10000E+01 volume

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0.111278+02

0.10000E-01 volume

. 897 ppm2

PP.

7.970 ppm2

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0.10000E+01 volume

7.970 ppm2

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0.786715.03

6.900 ppm2

0.18744E+04 ppm1

0.10000E+01 volume

7.689 ppm2

2

1.611 ppm3

volume

7.539 ppm2

Ppm1

0.182788.04

0.10000E+01 volume

7.714 ppm2

0.48715E+03 ppm1

0.10000E+01 volume

HEN)
WELGHT
HEN)

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10000	0.100001.0	0.100001	0.10000E+01	0.100005+01	0.10000E+01	0.10000E-01	0.100008+01	0.10000E+01	0.10000E+01	0.10000E+01	100008+01	.100008+01	.100008+01	0.100005+01	0.10000E+01	0.10000E+01	0.100006+01	0.10000E+01	0.100006+01	0.10000E+01	.100000.	10000	10000
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900	reeld 33 reeld 33	reeld 12 reeld 12 2.000 p	resid 107 and resid 103 and 2.200 pask	resid 14 and resid 102 and 1,600 peek	resid 34 and 1 resid 102 and 2.100 peak	resid 34 resid 98 2.200 g	resid 107 resid 79 1.300 pe	* 7 9	4 t 5	2000	4 32 6 32 0 0 0 0	aid 34 and a bid 102 and 2.100 peak	aid 107 and eid 110 and 2.000 peak	1.700 peak	resid 107 and r resid 107 and r 1.300 peak	resid 105 and r resid 105 and r 1.300 peak	d 34	A 4 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	reeld 102 2.300 p	# # 00 m	resid 103 2.100 P	770	14 34 14 61 1.200
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0.42209E+03 ppm1

0.10000E+01 volume

7.901

7.719 ppm2

0.35620E+03 ppm3

0.100008+D1 volume

0.10000E+01 volume

7.714 ppm2

1.641

Candq 689.7

0.44171E+03 ppm1

0.10000E+01 volume

0.10000E+01 volume

4.538

7.650 ppm3

2.6 1.13

7.646 ppm2

0.17361E+03 ppm1

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1.368

7.647 ppm2

0.42175E+03 ppm]

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1.706

7.616 ppm2

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0.10000E+01 volume 0.29483E+02

3.106

7.611 ppm2

0.10000E+01 volume

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2.374

7.611 ppm2

0.54543E+03 ppm)

0.100008+01 volume

1.496

0.16991E+03 ppm1

7.611 ppm2

0.400488+03 ppm)

0.10000E+01 volume
0.10000E+01 volume

3.30

7.535 ppm2

0.10679E+03 ppm1

0.10000E+01 volume

7.541 ppm2

0.21619E-04 ppm1

0.100008+01 volume

0.10000E+01 volume

7.529 ppm2

7.530 ppm2

0.46858E+03 ppm1

0.10000E+01 volume

0.10000E+01 volume

3.919

7.524 ppm2

3.70

7.524 ppm2

T M

0.10000E+01 volume

7.940

7.513 ppm3

volume

1.545

7.318 ppm2

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0.10000E+01 volume

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7.270

0.17762E+03 ppm1

0.10000E+01 volume

A651	Assi	AS81	1884	NBSI 1		7881 1881	5	¥ = -	A581		A8	- a	E	ASSI	Year -	E94	==	is	ASSI () 1884 ()	1884) 1884) 1897	VS81	֓֞֞֞֞֞֞֞֞֞֞֞֞֞֞֓֞֞֞֞֞֞֞֞֞֞֓֞֓֞֞֓֞֓֞֞֞֓֞֡
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	0.100	0.100	0.100	0.100		0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.100	,001			0.1000	0 . 1000	0.100005.01	0.100005+01	0.10000\$+01	o 1000001 o	
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D&Me 118.00 32.24	22.5	3 8	Dame H	name name 1111	name H	1354 V	3 3 4 4	115	115	11:	Dame H	name H	7524 V	name H name H 3574 v	7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2		Dene H		3804 V		1024 M	Dame Hi name Hi 4054 ve	Dame H	
and resid 82 and and resid 103 and 1.400 2.400 peak		resid 82 and n resid 81 and n 2.300 peak 3	\$ 4 4 5 5 4	2	9 6	\$ \$ ¥	111	resid 82 and resid 102 and 2.100 peak	F 5 5	4 4 4 4 4 4	\$ \$ 4		sid 82 and r aid 78 and r 2.000 peak	334	2 5 4 2 5 4	\$ \$:	resid 67 and r	A P	2.400 peak 3	2.100 peak	Pa and	Per share	a bud a	2 5
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2.400	P 0 0	2.600 and	2.400	2.400 and	D 0	11 17	2 2	2.100	9 9 9	9 9 0	9 9 0	778	2 4 8	2 4 8	P 200	9 2 8	2 2	9 g	# 0 E	8	2 2 8	110	B 5 0	
66.	2.600	22	66.	66	66	6.2	67. 2.20	997	99	66	2.100	die	66.	2.000	66.	66	66	2.900 rd • enc	6.	 	6 6 6	66.	55 5.1	66
3224 916 100 100	egid BrD and egid BrD and 200 2.600	egid 'BrO ' and egid 'BrO ' and .200 2.600	egid BrD and egid BrD and	eegid 'BrD and segid 'BrD and 3.100 2.400	megid 'BrD ' and megid 'BrD ' and	914 BrD	Megid "BrD " and Megid "BrD " and 1,000 2,200 3404)	Megid BrD and Megid BrD 2.100	megid BrD mand resid so and n megid BrD mand resid 102 and n 2.400 1.400 1.400 peak 3	egid "BrD and ingident and	segid BrD and resid 62 segid BrD and resid 78 2.900 2.100 2.100 pe	mgid "BrD " and resid 82 mgid "BrD " and resid 102 .300 2.600 2.300 p	egid Bro and a	egid BrD and segid BrD and 2.000	[1654] aegid "BrD" and reald 74 aegid "BrD" and reald 75 3.300 2.700 2.200 pm	1684} ggid "BrD" and resid 74 sgid "BrD" and resid 59 600 1700 1700	1754} mg1d *BrD * and r	3.400 2.900 { 3804} eegid "BrD " and	aegid "BrD " and r 3.100 3.400 [3944]	3.4024)	916 400 400 (\$20)	megid BrD and r aegid BrD and r 2.800 2.000	segid BrD and r segid BrD and r 2.300 1.300	(4204) segid 'BrD ' and segid 'BrD ' and
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1.00 1.10	7.714 ppm2	7.761 ppm2	7.802 ppm2			.03		4.026 pos2	•	4.023 ppm2	3.428 ppm3				!	6.179 DOM.	7.613 ppm2	7.680 ppm2	7.680 ppm	2.547 ppm2	2.548 ppm2	2.536 ppm2	2.548 ppm2	2.547 ppm2	. 007 pp
1.100 1.100 2.100 park 4104 weight 0.1000E-01 volume weight 1.00 1.000 park 4104 weight 0.1100E-01 volume weight 4.00 1.000 park 4104 weight 0.1100E-01 volume weight 4.			3							.163748.03	168316.03					0.15413R.03 ppm1									3.14312E+02 ppm1
### 100 pank 4104 weight ### 120						11000E-01 volume					-							volue	vol une	volume	volume	volume	volume	volume	vol te
3.100 3.100	1204 weight	name KKN) name KN)) 1264 weight	name KD\$) name KD\$) 1304 weight	name HZ)) name HA))	NAME HEL) NAME HEZ))	same HA1 1) same HO16) 5 weight	11	16 to 1 () 16 to 1 () 16 to 17 to		Lame HA1)) Lame HB4) 25 weight	name MB2 1) name MB1) 35 weight	Anne KB2)) Anne KO16) 45 weight		name HB2)) name HG2%) 55 weight 0.	11	Anne KDL 3) Anne KB4 3 65 waaght	name KD2)) name KB1) 75 weight	NAME HD2 })	name HD2)) name HD20) 95 weight	name HAN) name HG2N) 105 weight	name HAt) hame HG14) 115 weight	neme KAN) neme HBN) 125 weight	name HAN) name HA)) 135 weight	name HA1) name HA)) 145 weight	name KA1)) hame HE4)
	0 2.100 pesk	nd resid 34 and resid 31 and resid 31 and	nd resid 107 am nd resid 106 am 0 2.000 peak	nd resid \$2 and resid 103 and cast 2:200 peak	nd resid 107 and nd resid 76 and 7	od resid 201 and od resid 38 and 3	resid 201	nd resid 201 and nd resid 36 and 1.700 peak	** id 201	id resid 201 and id resid 43 and	id resid 201 and id resid 43 and	d resid 201 and id resid 36 and	resid 201 resid 34	d resid 201 and d resid 38 and	resid 201 resid 18	d resid 201 and dresid 43 and	::	d resid 201 and dresid 38 and	2.2	d resid 200 and d resid 38 and 1.700 peak	d resid 200 and d resid 38 and 1.400 peak	d resid 200 and d resid 43 and 1.800 peak	d resid 200 and d resid 38 and 1.700 peak	d resid 200 and d resid 43 and 1.800 peak	
				segid BrD at	(4364) segid 'BrD ' at segid 'BrD ' at 3.400 2.900	2.600	D100	2.400	megid Ack as	aegid "AcM" at aegid "BrD ar 2.600 1.700	- 4 4 4-	amgid "AcH a.m. amgid "BrD an 2.700 1.800	91699	segid 'AcH an megid 'BrD an 2.600 1.700	segid 'AcH an	eegid BrD an				aegid "Ack an aegid "BrD an 2.600 1.700	aegid "AcH an aegid "BrD an 2.400 1.400		megid "AcH " an aegid "BrD " an 2.600 1.700 [145]	aegid "Ack an segid "BrD and 2.700 1.800	segid "Ack " an aegid "BrD " an 2.700 1.800

7.461	7.401	7.637	7.637	7.585	7. 58 2	7.585	7.358	7.350	7.35	7.358	7.358	7.358	7.358
4.015 ppm2	3.429 ppm2	4.015 ppm2	3.429 ppm2	4.015 ppm2	3.429 ppm2	3.542 ppm2	4.019 ppm2	3.430 ppm2	3,430 ppm2	3.430 ppm2	3.430 ppm2	3.430 ppm2	3.430 ppm2
0.13824E+03 ppml	0.15229E+03 ppm1	0.18465E+03 ppm1	0.13938E+03 ppm1	0.16075E+03 ppm1	0.16293&+03 ppm1	0.14049E+03 ppm1	0.16796E+03 ppml	0.16763E+03 ppm1	0.12000E+03 ppm1	0.12000E+03 ppm1	0.12000K+03 ppm1	0.120008+03 ppm1	0.12000E+03 ppm1
0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 valume	0.11000E+01 volume	0.11000£+01 volume	0.11000E+01 volume	0.11000E-01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 volume	0.11000E+01 Volume	0.11000E+01 volume	0.11000E+01 volume
6 and name 6 and name 01 and name 5 and name 0 peak 16	resid 301 and name KD1) resid 35 and name KD1) resid 301 and name KB1) 1.700 peach 26 weight resid 301 and name KD2) resid 301 and name KD2) resid 301 and name KD2)	resid 201 and name MA1) resid 88 and name MD3) 1.600 peak 36 weight resid 201 and name MA2) resid 80 and name MD1)	resid 201 and name HB2 1) resid 84 and name HDb) 1.800 peak. 46 weight resid 201 and name HB1 }) resid 88 and name HDb)	reald 301 and name HA2)) reald 95 and name HS1) 1.700 peak 56 weight reald 201 and name HA1)) reald 95 and name HE1)	and name and name	resid 300 and name HAN) resid 95 and name HEN] 1.800 peak 76 weight	resid 201 and name HA1)) resid 88 and name HE1) 1.700 peak 6 weight resid 201 and name HA2)) resid 88 and name HE1)	Testd 201 and hame HB2)) Testd 88 and hame HB1) 1.700 pesk 96 weight Festd 201 and name HB1))	and name and name ax	iresid 200 and name HAt) I resid 201 and name HAI)) 1.800 peak 17 weight	HB2)) HD1)) weight	name HD1)) name HB1)) name HB1)) name HB2)) name HB2))	resid 201 and name HAZ 1) 1:400 peak 47 weight (resid 201 and name HAI 1) resid 201 and name HAI 1) resid 201 and name HAI 1)
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Ambiguous NOE-derived Inter-proton Distance Restraints

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		1.738 ppm2			9.740 00=2					666				6.673 ppm2				7.977 ppes2									8.612 5093					rudd ont					, ,	Turk here					
		-03 ppm1			03 ppm1	ł				100	į			02 ppm1				03 ppm1																									
		he 0.35526E+02 ppml			* 0.20417B+03 ppm1					e 0.15089E+03 pom;				. 0.45645E+02 ppm1				# 0.17645E+03 ppm1									0.12021E+02 ppm1	•			0.63178E+01 nmm1						0.12608E+03 com1						
		0.10000E+01 volume			0.10000E+01 volume					0.10000E+01 volume				0.10000E+01 volume				0.100008+01 volume									0.10000E+01 volume				0.10000K+01 volume						0.10000E+01 volume						
			KN)	11		22		==	=	MA 1) weight 0.1000		Ξ	KN)) HB2))		HN 11	= :	HB1))		= :	=	==	: :	==	=	2	==		=	: 2	=		=	:=	=	_	= :			: _	=-	=	_	22
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	freeid 32 and resid 35 and	1.300 pe	resid 28	seid 106	2.400 P	resid 106 .				2.200 peak	esid 100	9 PT 9	16 pre-	Z.			resid 97	2.300 peak	resid 78 av		resid 79 at	2				reeld 76 an	X.	resid 76 and	resid so an		0.000 peak		resid 72 and			resid 21 and	Z	eid 21 and	resid 106 and	resid 109 and resid 106 and	resid 64 and		resid 26 and resid 22 and
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2.672	3.631		2.10	***	•	2.36		2.204	3.072
9.196 ppm2	1.763 ppm2	6.794 ppm2	6.809 ppm2	6.810 ppm2	9.156 ppm2	6.663 ppm2		6.133 ppm2	6.574 ppm2
0.12549E+03 ppm1	0.14751E+03 ppm1	0.41938E+02 ppm1	0.402028.02 ppm1	O.672416+02 ppml	0.54619E+02 ppm1	0.24821E-03 ppm.1 0.98690E-02 ppm.1		0.55139E+02 ppm1	0.12194E+03 pps.1
E 0.10000E.01 volume	0.10000E.01 volume	0.10000E+01	0.1000E.01 volume 0.1000E.01 volume	0.10000£.01 volume	0.10000E+D1 VOLUME	D.10000E.01 volume		0.10000E.01 volume	0.10000E+01 volume (
eak 1781 weight and name MB)) and name MB)) and name MB))	k 2721 nd name nd name	and name and hame ak 1261 and name and name and name	and name HN)) and name HN)) and name HOJ)) peak 1371 weight and name HN)) and name HOJ))	and name NN)) peak 3401 weight and name NO)) and name NO)) and name NO)) and name NO))	A name HN A name HB1 3671 weigh	o and name (M)) peak lets waight and name (M)) and name (M)) and name (M)) and name (M))			name NB2)) name NB2)) name NB)) name NG2)) 6861 weight
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1.400 2.3 (1 1781) (1 megid "BED - (1 megid "BED -	1.300 2721) eegid 'BrD - 2721) eegid 'BrD - eegid 'BrD - eegid 'BrD -	2014 '810 1261	1361) 1361) 1370 1370 1371) 140	(eegid 'BrD ' and leegid 'BrD ' and little 1401 1.600	2000 1000 1000 1000 1000 1000 1000 1000	9891d 9875 - 3841) - 3841) - 3841 3841 3841 3871 3	megid Tarb and	### ### ### ### ### ### ### ### ### ##	### ### ##############################
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	- 2	P 6 6			and hame					8		rD and resid a	and bas	
	~ ~ ~ .	1.300 ( 6071)	2.70d	17 7	Peak 6871			8.573 ppm2	2.703	7		rD and resid 3	and name	3 2
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	;===	9.91d	Brb . ank	resid 89 resid 85	and name and name tak 7121	0.10000E+01 volume			į	)	89914 Br	O and resid Se O and resid 35	and name	
1.10   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20   1.20	_===	0.00 d	Bro . and	reeid as	and name			Zwdd F76:	5.021	) NO	Begid "Br 3.600	1.200 1.900	and name	M01 ))
11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.11   11.1	:==	3.600	BrD and BrD and	resid 89	and name						megid "Br eagid "Br { 8691}	D and reeld 9		18 H
	~==:	11111 6916 •	BrD . and	reald 69	and name	C. LOCOUL+UI VOLUMA		8.416 ppm2	5.021		4.000	0 * And resid 10	1	H ight
	: = =	piga.	Bro . and	racid 26 recid 22	and name						eegid "Br eegid "Br { 8901}	D * and resid 11	2 and name HM 3 and name HA	==
10   10   10   10   10   10   10   10	-=-	7251)	2.200 BrD * and BrD * and	2.200 reeld 26 reeld 56	ek 7251 and hame and name	0.100008+01 volume		9.196 ppm2	1.549	55 5	megid "Br eegid "Br 3.400	D * and resid 11: D * and resid 10 2.900 2.100	and name and name	KM )) KA )) veight 0.100
9916 'BD' and reald 57 and reald 57 and reald 59 and reald 59 and reald 59 and reald 50 and reald 59 and reald 50 and real	==	egid "	BrD and BrD end	resid 57 resid 25	and name and name ak 8181					8	991d 'Br	99	and name	==
		8101) 891d -	arb . and	resid 57	and name			9.159 ppm2	1.667		egid *Br	9	and name KN	==
132   132   132   132   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133   133		8181) 8691d %	Per Co.	reald 57	and neme						Megid *Bri Megid *Bri 3.500	3.100 2.000	and name and name peak 4911	HM )) HA )) weight 0.1000
1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00		1 page 1	ard and	resid 114	and name HN ))					1))	segid Bri	and resid 112	And name HM	==
10   10   10   10   10   10   10   10		8211) eegid :	61. 61. 61. 61. 61. 61. 61. 61. 61. 61.	1.500 resid 114 resid 119	ak 8211 weight and name HN ))	0.10000E+01 volume	0.47918B+02 ppm1	6.377 ppm2	2.37		egid Bri	2.100 2.100	and name HN )) and name HBt ) peak 8941 weight	٠ ۽ ۽ ۽
1,014		1 p161)	aro and 1ro and 4.200	resid 28	and name KN ))					8	egid Br	22	and hame	==
( seed 28 and name RN )		1261) eegid 1	tro and	reeld 28	nd name KN ))	Service to the control of the contro	0.16987B+02 ppm1	8.166 ppm2	3.014		egid 'BrD 9011}	::::	and has	== :
## And resid 28 and name H21 ))  **Sedid "BIO" and resid 28 and name H21 ))  **Sedid "BIO" and resid 28 and name H21 ))  **Sedid "BIO" and resid 105  **Sedid "BIO" and resid 105  **Sedid		4.400	10 . and	resid 26 rasid 25 1.100 p	nd name RN }) and name HG24) ik 8291 weight	3.10000E+61 volume		3			.100 .100 011}	00 g	and name	
		1. piges	a a	resid 28	7.6 mg					Y Y	9914 '6rD 9031) Agid '8rD	\$ 5 E	and name HB1 ))	: 2

1.674	9. 00.	2. 6 4. 6 4. 6	2. 747	1.61	4.81	. e . e . e . e . e . e . e . e . e . e	*	2.17g	3.294	1.80\$
6.743 ppm2	6.743 ppm2	8.564 ppm2	10.051 ppm2	9.052 ppm2	4.668 ppm2	4.668 ppa2	6.668 ppm2	8.667 ppm2	8.447 ppm2	8.447 ppm2
0.13119E+O3 ppm1	0.452116+02 ppm1	0.702108+03 ppm1	0.128118-03 pps1	0.861538+02 ppm1	0.44524E+02 ppm1	0.112798.03 ppm1	0.107628+03 ppm1	0.29817E+03 ppm1	0.22428E+03 ppm1	0.623318-02 ppm1
0.10000E+01 Volume	0.100006+41 volume	0.100006.01 volume	0.10000E.01 volume	0.10000E+01 volume	0.100005.01 voluma	0.10000E+01 volume	0.1000DE+01 volume	0.100005.01 volume	).10000E+01 volume (	0.10000E+01 volume d
"BTD" and resid 61 and name HAW )) "BTD" and resid 59 and name HOZ9) 3.900 2.100 pask 8351 well "BTD" and resid 61 and name HAW ) "BTD" and resid 22 and name HAW )	The state of the s	1.000 Period 50	and resid 44 and name HH	resid 3 and name resid 8 and name 3.900 peak 861 resid 9 and name resid 7 and name	ceid 103 and 1.500 peak 1.500 peak ceid 112 and ceid 113 and ceid 113 and	and resid 112 and name (kt ))  90 2.100 peak 8001 weight and resid 103 and name (kt ))	and resid 101 and name and resid 100 peak soll like 2.000 peak soll like resid 112 and name and resid 110 and name	Mad resid 100 and nesses HP 1)  20 2.100 peak 8941 weight  Ind resid 101 and name HP 1)  Ind resid 102 and name HP 1)  Ind resid 102 and name HP 1)  Ind resid 102 and name HP 1)	ind resid 105 and name to force and 104 and name 10 2.400 peak 911 und resid 105 and name ind resid 103 and name	and resid 105 and name NN )) and resid 102 and name NB2 )) do 1.700 peak 9031 weight
( eegid 'BrD • ( eegid 'BrD • 2.9 OR ( 8381) ( eegid 'BrD • ( eegid 'BrD • ( eegid 'BrD • ( eagid 'BrD • ( eagi		( eagld 'BrD ' ( eagl		A651 [ 884.] ([ 8691d 'BrD   1,600.] ) G 864.] OR [ 884.] ([ 889.4 'BrD   1,600.] ([ 889.4 'BrD   1,600.] A53. [ 883.1   883.1			6911   6911   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   6921   69	######################################		( espid BrD

c	•	7

7			•		. 4					6.55						25.4										. 63	
0.13642E+03 ppm1			0.35471E-02 ppm1		0.30219E+03 ppm1		0.12105E+03 ppm1			0.555056+02 ppm1		0.53501E+02 ppm1				0.72347E+02 ppm3		0.141316.0					tedd roses or			0.86367E+02 ppm1	
0.10000E+01 volume			0.10000E+01 volume		0.10000E+01 volume		0.10000E+01 volume			0.10000E-01 volume		0.10000E+01 volume				0.10060£+01 volume		0.10000E+01 wolume				0.10000E-01				0.10000E+01 volume	
peak 9261 weig	107 and name HN 1)	1 1	\$ Î	14 and name HN ))	13 and name HN )) 14 and name HEV ) 10 peak \$141 waight	12 and name HM 1)	12 and name HN )) 14 and name HGZ () 10 peak 9371 weight	2 and name KW ))	and name	teld 109 and name HB )) teld 109 and name HB2 )) 1.600 peak 9441 weight	and name	1 and name HW )) 4 and name HG2 )) 0 peak 9451 weight	1 and name HW 1)	1 and name HW )) 3 and name HG1 ))	1 and name HN ))	4 and name HN )) 1 and name HBI )) 0 pnak 9461 weight	1 and name HW )) 3 and name HB2  )	1 and name HN )) 9 and name HB2 )} 0 peak 9491 weight		and name	4 and name HN ))	and name and name peak 9501	11	and name	and name HM ))	and bear	and name KN
3.700 3.200	wegid "BID" and reald 84 9281} eegid "BID" and reald 63 eegid "BID" and reald 63	( aegid "BrD" and reald 22 and na	4.200 1.30	d "BrD " and reald e d "BrD " and resid a	({ eegid "BrD" and resid 63 and na ( segid "BrD" and resid 74 and na ( 2.90 2.100 2.100 peak 93 ( 9341)	d 'BrD ' and reeld 2 d 'BrD ' and reeld 1	(( aegid 'BrD' and rasid 22 and na (( aegid 'BrD' and rasid 24 and na 12.400 2.900 2.100 peak 93 ( 9371)	eegid "BrD " and resid 22 megid "BrD " and resid 23 9371]	aegid BrD and reald 63 eegid 83 and reald 59		segid "BrD " and resid 64 aegid "BrD " and resid 64 [ 9451]	megid BrD and resid 21 megid BrD and resid 24 3.900 3.800 1.600 1	segid "BrD " and resid 21 aegid "BrD " and resid 24	eegid "BrD " and resid 21 megid "BrD " and resid 23	1 BrD and reeld 2	() Segid "BrD" and resid 64 and name Hb () Segid "BrD" and resid 61 and name HE 3.700 3.400 1.800 peak 9461 we	1 'BrD and resid 2	( aegid 'BrD " and reaid 21 and nes ( aegid 'BrD " and reaid 19 and nes ( 3.100 2.700 2.200 peak 948	( segid 'BrD . and resid 109 ( segid 'BrD . and resid 111	"BrD " and reald 109	"BrD " and resid 64	[ 9501] aegid "BrD" and reaid 21 and resid 27 and resid 27 and resid 37 and resid 37 and resid 2.700 and resid 2.200 peak 9	bra . Gra.	or o	*BrD * and resid 17	Ora.	Bro . ord
3.30 08 ( 928)	OR ( 92914 ( 89914 ( 89914	1884 ))	2.30	bigee )) bigee )) bigee )) bigee )	( eegid ( eegid 2.900 OR ( 9341)	( sagio ( segio A591 ( 917	(( eegid () eegid 3.400		(( aegid ( aegid ASSI ( 944	(( segid () segid ).900 OR ( 9441)	(( aegid (( aegid ASSI ( 945	), piger ))		( segid	D1600 ))	( megid ( megid ( megid 3,700	piges ))	). 3.300	OR ( 9491) (( aegid (( aegid	pige )					(rect   lead (rect)   (rect)   (rect)	OR ( 9531)	OR ( 9531) (( megid (( megid
																										۰	<b>.</b> -
	3.674					2.48		1.725		2.560		2.316				2.150		2.003		1.786		3.908		2 352			
	6.574 ppm2					4.573 ppm2		8.574 ppm2		9.740 ppm2		9.739 ppm2				9.742 ppm2		9.740 ppm2		9.739 ppm2		9.464 ppm2		9.463 pom2			
	0.66318E+02 ppm1					U.Jottekedi ppmi		0.10029E+03 ppm1		0.56197&+02 ppml		0.47295E+02 ppml				0.40041E+02 ppm1		0.15794K+02 ppm1		0.56492E+02 ppm1		0.69670R+02 ppm1		0.78060E+02 ppm1	:		
	0.10000K+01 volume							0.100008+01 volume		0.10000E+01 volume		0.1000dE+01 volume				0.10000E+01 volume		0.10000E+01 volume		0.10000E+01 volume		0.10000K+01 volume		0.10000K+01 volume			
and name HN ))	and name HN )) cand name HB2 )) peak 9091 weight	and name HN 1)	and name HN ))	and name HN	and name and name	1	and name HN and name HO2	and name	and name	peak 9161 and name	and name	peak 9171	end name	and hame	and name	peak 9161 weight and name HN  )	and name	and name xeak 9191 and name	1	9201 9201	Deme	and name HW }} and name HD2 }} peak 9241 weight	and name KN ))	and name HN )) and name HG1 )) peak 9251 weight	and name	and name HB1 ))	and name KN 11
eegid "BrD " and resid 105	1 8rD * and reaid 109 1 8rD * and reaid 106 1 3.600 1.700 p	"BrD * and resid 109	"BrD " and resid 109	"BrD " and resid 64	and reald 64 and reald 63	eaid 21	reald 21 reald 17	01 P144	segid BrD and resid 106 and segid BrD and resid 104 and	3.900 3.850 1.600   9161)   4691d *8rD * and resid 106   4691d *8rD * and reaid 103	( 9171) eegid 'BrD ' and resid 106 eegid 'BrD ' and resid 109	1.500	9171) segid BrD and resid 106	9171 9201 BrD and resid 106		eegid BrD and resid 102 and 4.100 1.400 peak 9181] and resid 106 and	eegid BrD and reaid 106 and	4.200 4.200 1.300 9191) 9191) 9201 9201 9201 9201 9201 9201 9201 9201	eegid "BrD " and resid 109 { 9201}	7.800 1.600 peak	segid BrD and resid 106 and segid BrD and resid 25 and { 9241}	rD * and resid 84 rD * and resid 80 3.400 1.800 p	20 pt 0	(( aegid "BrD " and reald 63 (( aegid "BrD " and reald 62 3.700 3.400 1.800 p	rD * and resid 64.	degid 'BrD " and reald 84 eegid 'BrD " and reald 86	rD * and reald 84
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9.462 ppm2

4.67

9.472 ppm2

7.530

9.456 ppm2

3.066

9.456 ppm2

2.173

8.557 ppm2

3.108

8.556 ppm3

2.851

8.544 ppm2

1.929

4.556 ppm2

1.763

0.556 ppm2

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6. 695 ppm2

1 0.666 ppm2	1 6.785 ppm2				11 7.596 ppad	7.596 ppma
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3.661	4.94	1.920	3.146	3.659	2.384	1.13
6 . 634 ppm2	6.936 ppm2	6.936 ppm2	6.566 ppm2	6.669 ppm2	6.668 ppm2	6.669 ppm2
0.155048+03 ppm1	0.54041E.02 ppml		0.46621E+02 ppm1	0.19838E+02 ppm1	0.70791E+02 ppm1	0.244198-03 ppm1
0.100008.01 volume	0.10000K.01 volume	0.10000E.01 volume	0.10000E+01 volume 0.10000E+01 volume	0.10000E-01 volume	0.100006.01 volume	0.100008.01 volume
Dames HN )) Dames HB )) 9561 weight names HB )) names HB )) names HB )) names HB ))	and name HN )) peak Still wight and name HL )) and name HB )) and name HB )) and name HB Still S	and name HO1 )) and name HO2 )) and name HO3 )) peak \$61 waight and name HO ))	and name HW ))  ak 9721 weight  and name HW ))  and name HB ))  and name HB ))  end name HE ))	11d 23 and name 12d 1) 11d 22 and name 12d 1) 11d 100 and name 12d 1) 11d 100 and name 18d 1) 11d 100 peak \$801 asight 11d 100 and name 18d 1) 11d 13d and name 18d 1) 11d 13d and name 18d 1) 11d 02 and name 18d 1) 11d 02 and name 18d 1)	resid 103 and name NH 1) resid 10 and name NH 1) resid 11 and name NH 1) 1.800 pack 9521 velight resid 11 and name NH 1) resid 12 and name NH 1) resid 11 and name NH 1) resid 12 and name NH 1) resid 13 and name NH 1) resid 14 and name NH 1) resid 14 and name NH 1)	and hase and name and name and name and name and name and name and name and name and name and name
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901) 9914 *BrD 10981) 9914 *BrD 9914 *BrD 9914 *BrD				1121) 1121) 1121) 1121) 1121) 1210 1210			
OR [10901] ( segid "BrD ( segid "BrD ( segid "BrD ( segid "BrD ( segid "BrD ) :500 OR [10981]	(6 aegid 'BrD (7 aegid 'BrD (7 aegid 'BrD (7 aegid 'BrD (7 aegid 'BrD (7 aegid 'BrD (7 aegid 'BrD	ASS: (1718)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)   (1884)	(( megid "BTD ASS (11271) (( megid "BTD ( megid "BTD ( megid "BTD ( 11271) (( megid "BTD ( megid "BTD ( megid "BTD ( megid "BTD ( megid "BTD ( megid "BTD ( megid "BTD	0.0 (11301) (( eegdd 'BED (11301))	( 1889)4 'BED (	(( eegid "Bro ( ee	10.500 (1.16.1) ((.eegid 'BFD') ASS (1.14.1) ((.eegid 'BFD')
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ppm3	Çwed	Zwdd		ppm2	pps:	ppm2	8.005 ppm2
7.984 ppm2	7.974 ppm2	7.974 ppm2		7.975 ppm2	9.680 ppsů	8,004 ppm2	8.005 ppm2
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2 g	0.427266+03 ppm1	0.11084E.03 pps1		0.13251K-03 ppm1	0.21458E+03 ppml	0.57791E+02 ppml	0.948058-02 ppm1
3692	7366	10 40 00		22 5 3 E	14585	7791E	10058
2.							ě. 0
0.10000E+01 volume 0.52287E+03 ppml	0.10000E+01 volume	0.10000E+01 Volume		0.10000E+01_valume	0.100008.01 volume	4.10000K.01 volume	0.10000E+01 volume 0.94605E+02 ppm1
8	5	\$		8 .	8 8	10	5 5
000K+	0006	<b>.</b>		600F•	000 E+	000E+	000 E.
o.1	9.10	0.10		0.10	0.10	0.10	0.10
HR CAST	== == # =:	HA )) HO20) HO20) HO10) HO10) HO10)	H	HN )) HN )) HN )) HN )) HN )) HN ))	HM ))	HW )) HW2 )) V419ht HW )) HW1))	HB2 )) HG1() HG1() HB2 )) HB2 )) HG1 )) weight
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0.123266.03 pps.1	0.169026.02 ppm1	0.42662E.02 ppm1	0.47235E+02 ppm1	0.60\$27E+02 ppm1	0.37827&+02 ppm1	0.26537E-04 ppml
0.100006.01 volume 0.13346.03 ppsi 0.100008.01 volume 0.680308.02 ppmi	0.100008+01 volume 0.369026+02 ppm1	0.10000E.01 Volume 0.42642E.02 ppm1	0.10000E+01 volume	0.10000E.01 volume	0.10000E+01 Volume 0.37827E+02 ppm1	0.100006.01 volume 0.26537E.04 pgml
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6.218 ppm2

0.10000E+01 volume 0.16014E+03 ppm1

1.664

8.047 ppm2

0.10000E+01 volume 0.28782E+02 pps1

4.526

4.087 ppm2

0.10000E+01 volume 0.41005E+02 ppm1

2.695

0.631 ppm2

0.10000E+01 volume 0.37922E+02 ppm1

4.880

9.167 ppm2

0.10000E+01 volume 0.59211E+02 ppm1

1.737

8.669 ppm2

0.100005+01 volume 0.30609E+02 ppm1

3.346

0.10000E+01 volume 0.79191E+02 ppm1 6.960 ppm2

1.797

6.980 ppm2

0.10000K+01 volume 0.35919K+00 ppml

2.529

6.522 ppm2

0.10000E+01 volume 0.42059E+02 ppm1

1.422

4.521 ppm2

0.10000E+01 volume 0.52230E+02 ppml

2.111

6.522 ppm2

0.10000E+01 volume 0.41867E+02 ppm1

6.56 ppm2	8.565 ppm2	9.473 ppm2	6.377 ppm2	5.742 ppa2	6. 685 pp.2.	9.156 ppm2
0.100006:01 volume 0.178095:03 ppm.i	0.10000E.01 volume 0.81304E.03 ppm1	0.10000E.01 volume 0.4890E.02 ppm1	0.100006.01 volume 0.14455.02 ppm1	Volume 0.20479E+02	0.10000E+01 volume 0.92105E+02 ppm1	0.10000E:01 volume 0.4946E:02 ppml
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0.41415E.	0.23452E+03 ppm.1	0.130\$58+03 ppm1	0.540955.02 ppm1	0.10060E.03 ppm1	0.10295E+03 ppm1	0.611648+03 ppml
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ABBI	:: <del>1</del> :	- EST - E	5 38 5	- B	7 7 18 V881	5 8	8	22.8	=_ ;		1==	ਰ = _ ਵ	5	7 F	8	7	8 3	8 8		:	1 = =	8	7 × ×	5	<b>188</b>
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8.566 ppm2

PPM1

volume

And the second control of the second control

8.568 ppm2

volume

1.576

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volume

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7.974

4.494 ppm2

volume

and name and

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0.24650E+02 ppm1

3.965

9.035 ppm2

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0.259488+02

vol une

1.041

2 1.037

. 25

0.12633E+02 ppm1

we ight ¥ 5 7.621

4.680 ppm2

0.10000E.01 volume

and name Ki and name K is and name K be and name b

8.858 ppm2

4.762 ppm2

(( sagid "BrD" and reald 15 ASS (11558)	BrD and BrD and BrD and BrD and 2.100 BrD and BrD and BrD and Company BrD and	Bro and 2,200		Assi ( segid 'BrD' and resid 9)	segid 'BrD and 2.500   1702   1702   1703   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704   1704	(( eegid 'BrD' and resid 5)  ( eegid 'BrD' and resid 0)  ( eegid 'BrD' and resid 0)  ( eegid 'BrD' and resid 4)  ( eegid 'BrD' and resid 4)  ( eegid 'BrD' and resid 1)
1.110	1.643	1.601	5.288 6.147	1.642	1.430	3.441
1 8.004 ppm2	8.562 7.735	1 13.275 ppm2	. 640 ppm2	1. 9.077 ppm2	6.731	41 6.809 ppm2
0.20319R+01 ppml	0.116158-03	0.50580E+02 ppml	0.221855.02 pps.l	. 0.294416+02 pps1		e 0.115962.03 ppml
6.10000E-01 Volume	0.10000E+01 volume	0.100008+01 volume	0.100005.01 volume	0.10000E+01 YOLUMA	0.10000E-01 volume	0.10000£.01 volume
1516 54 and name (NY ) 1516 12 and name (NO N) 1516 12 and name (NO N) 1516 152 and name (NO N) 1516 152 and name (NO N) 1516 152 and name (NO N) 1516 153 and name (NO N) 1516 153 and name (NO N) 1516 153 and name (NO N)	and hame and name	and name	and name HN and name HBy and name HW and name HB and name HB and name HB peak 15341 wai,	and name (NY )) and name (NY )) peak 15411 wight and name (NY )	and name HN )) and name HR ) and name HD38) posk 12461 weight and name HB )) and name HB ))	and name and name and name and name and name and name and name and name and name
		1.600 esid 30 esid 32 1.300 1.300	TO and resid 25  TO and resid 25  TO and resid 25  TO and resid 27  TO and resid 24  TO and resid 24  TO and resid 24  TO and resid 24	ser	914 'BrD' and readd 106 (1841)   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840   1840	resid 14 resid 15 0.500 resid 15 resid 15 resid 14 resid 14 resid 15 resid 15
Add "810" and r Add "810" and r (1 eagld "810") and r (1 eagld "810" and r (1 eagld "810") and r (1 eagl	0.8   1.400   2.900   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400   1.400	(1.514.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.) (1.624.)	( 1991 d' 910 e and ( 1992 d' 910 e and ( 1993 d' 910 e and (  1993 d' 910 e and (  1993 d' 910 e and (	ASSE (1541) (1 eagld BED end (1.300 BED end (1.341) (2 eagld BED end (1.341) (3 eagld BED end (1.341) (4.341) (4.341) (4.341) (6 eagld BED end (6 eagld BED end (7 eagld BED end (8 eagld BED end	(1 mag)	Assi (1549.)  Assi (1549.)  (1 00914 '970 'nnd  (2 00914 '970 'nnd  (3 00914 '970 'nnd  (4 00914 '970 'nnd  (5 00914 '970 'nnd  (6 00914 '970 'nnd  (7 00914 '970 'nnd  (7 00914 '970 'nnd  (8 0914 '970 'nnd  (8 0914 '970 'nnd  (8 0914 '970 'nnd  (9 0914 'nnd  (9

3.645 3.306 4.477 3.667 4.502 2. 179 1.994 4.985 2.779 1.057 ppm2 4.854 ppm2 2.190 ppm2 1.057 ppm2 2.291 ppm2 2.190 ppm2 1.054 ppm2 11.082 ppm2 1.057 ppm2 1.546 ppm2 3.289 ppm2 11.082 ppm2 3.373 ppm2 12 and name Hill)
13 and name Hill)
14 and name Hill)
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18 and name Hill)
19 and name

( megid "BrD * and resid 14 and hame HI (1221) ( megid "BrD * and resid 17 and name HI ( megid "BrD * and resid 109 and hame HI ( megid "BrD * and resid 109 and hame HI ( megid "BrD * and resid 109 and hame HI ( megid "BrD * and resid 109 and hame HI ( megid "BrD * and page 1 and hame HI ( megid 109 and hame HI )	HD16) HB )) HG1 ))				( segid 'B 2.600 OR ( \$712)	aegid 'BrD' and resid 102 and 2.600 1.700 1.700 pask 8712   and resid 56 and aegid 'BrD' and resid 56 and	22 and name HD1%) 2 peak 8712 weight 4 and name HD1%)	0.100005.01 volume 0.36561E-01 ppm1	0.26561E+03 ppm1
7232	0.10000E+01 volume	0.48663E+02 ppml	4.854 ppm2	4.37	OR ( 8712) (( segid *B ( segid *B ASSI ( 8962)				
DAMA DAMA DAMA	MB )} HD24) HG24)				(( segid 'B ( segid 'B ).700 OR ( 8962)	angid "BrD " and rasid 54 eegid "BrD " and resid 23 1,700 3.400 1.600	eid 56 and name MB2 )) eid 25 and name MG2) 1.800 peak 8962 weight	0.10000E+01 volume	0.31139K+02 ppm1
7262	t 0.10000E+01 volume	0.437128+03 ppml	1.747 ppm2	1.321	( megid 'B ( megid 'B ( megid 'B	segid "BrD " and resid 102 segid "BrD " and resid 101 89621	32 and name HB1 )) 31 and name HG2N)		
1	HG21)					segid "BrD" and resid 56 segid "BrD" and resid 22 ( 9112)	and name HB2 ))		
and name HU and name HC peak 7392 we	HA 1) HG 1) weight 0.10000£-01 volume	0.25131K+02 ppm1	4.605 ppm2	3.334	( segid '8 ( segid '8 2.600		eid 21 and name HO20) sid 102 and name HD20) 1.700 peak 9112 weight	0.10000E+01 volume	0.2659eK+03 ppm1
And name IV	HB 1)				e pifee )	segid 'BrD ' end reald 101	Di and name HG26)		
nd name nd name k 7742	HA )) HG14) Weight 0.100008+01 volume	0.51859E+02 ppm1	4.557 ppm2	1.417	8 936	segid TBTD end resid 21 and segid TBTD and segid BTD and resid 78 and 1,000 1,700 peak 1	1 and name MG24) 8 and name MD14) 9 peak 9142 weight	0.10000E+D1 volume	0.279688+02 ppm1
and of the same	HA 1)					segid 'BrD ' and rasid 31 segid 'BrD ' and resid 31	1 and name HG24)		
( segid BFD and resid 77 and name Hi ( segid BFD and resid 80 and name Hi 3.300 2.700 2.200 peak 8052 we	HB1      HB2      waight 0.100006.01 volume	0.59988E+02 ppm1	3.325 ppm2	2. 564		[ 5124] segid "BrD " and resid 21 segid "BrD " and resid 18 2.500 1.600	1 and name HD1%) 8 and name HD1%) 0 peak 9192 weight	0.100005+01 volume	0.360765+03 COR
nd name	ИВ1 3) НВ1 3)					segid "BrD " and rasid 21 segid "BrD " and resid 78	and name		:
and name Hi	HS1 ))				ASSI ( segid "BrD " and ( segid "BrD " and ( segid "BrD " and	rb and resid 79 and rr	11		
sid 63 and name HU sid 62 and name HI 1.800 peak 8123 w	HA   )     HB1   )     weight 0.10000E+01 volume	0.10661E+02 ppm1	5.296 ppm2	3.660	3.000 OR [ 9662) (( segid 'B (( segid 'B	3.000 2.200 2.200 ps62) pegid "BrD " and resid 79 aegid "BrD " and resid 116	D peak 9662 weight and name KG1 )) 16 and name KG11)	0.10000E.01 volume	0.10300E+03 ppm1
and name	HA )) HB2 ))				A8SI (10002) (( aagid "B ( aegid "B 3.600	881 (10002) ((aegid "BrD" and resid 54 and name (aegid "BrD" and resid 81 and name 3.600 3.800 1.900 mesk 10002	t and name KB1 )) 1 and name HG10) Deak 10002 enight	0.10000R-01	Sept. Of
2486	HA ))	-			OR (10002) (( eegid 'B	10002] eegid "BrD " and resid 42 segid "BrD " and resid 18	and name HB2 ))		
and name and name ak 8212	0.10000E+61 volume	0.72542E+03 ppm1	1.401 ppm2	2.310	Assi (10092) (( segid 'BrD ' and (( segid 'BrD ' and ),100 2.400	rD * and resid 35 rD * and resid 32 2.400 2.400	s and name HG1 )) 2 and name HA )) 2 reak 10092 seight	carlos to account of	
and name	HD24) HQ				OR (10092) (( segid 'B (( segid 'B	2.2	P P P P P P P P P P P P P P P P P P P		
	HA }) weight 0.1000E+01 volume	0.19700E+61 ppm1	0.414 ppm2	4.626	A881 [10182] ({ segid "B (( segid "B (.100	18 (10162) (( segid "BrD " and resid 52 (( segid "BrD " and resid 50 4.100 4.100 1.400	2 and name KB1 )) 0 and name KG1 )) 0 peak lois2 weight	0.10000E+01 volume	0,17\$26E+02 ppm1
and name K	MD21)				(( eegid 'B (( eegid 'B (( eegid 'B	ON (10102) ([ segid 'BrD * and resid 84 (  segid 'BrD * and resid 80 on reside 80 on res	4 and name KB1 )) o and name KO1 ))		
D and resid 71 and name H. D and resid 22 and name H.	HA 1) HD1(1)				( angld 'B ( angld 'B ( angld 'B	( eegid "BrD " and resid 42 ( eegid "BrD " and resid 39 ( eegid "BrD " and resid 39 3.000 2.200 2.200	and name HO1 }} and name HD1 }} beat 10302 weight	0.10000E+01 volume	0.106068.03
end neme	HBZ   }   weight 0.100008+01 volume   HD18.	0.24926E+03 ppm1	1.645 ppm2	4.629	08 (10302) (1 eegid '8 (1 eegid '8	22	and name and name		
and name H	HD ()				( segid BrD and ( segid BrD and ( segid BrD 2.000	rD * and resid 48 rD * and resid 48 3.000 2.000	raid 48 and name HA )) raid 46 and name HB1 )) 2.000 pask 10412 waight	0.10000£+01 volume	0.17461E+03 ppm1
	HD11)				8 biges ))	segid "BrD " and resid 87 segid "BrD " and resid 87 (1950)	and name HA ))		
Dem 0	0.300005.01	1074,077		90	( segid 8	( magid BrD and reaid 112 and name ( eagid BrD and reaid 111 and name 2,700 1.800 1.800 peak 10502	12 and name HB1 }) 13 and name HB4 } 0 peak 10502 weight	0.10000E-01 volume	0.19681E+03 ppm1
M seed bus				ئىر	bra " Graff "Bro " and " brad " Graff " brad " Craff " brad " bra	rD * and resid 112	12 and name HB1 )) 09 and name HD1 ))		
Į	(A10)			•	(10001) 1884 (10001) (10001) (10001)	(10602) eegid 'BrD' end resid 3) eegid 'BrD' end resid 19	and name HA ))		

3.621 ppm2

2.298

2.880 ppm2

2.762

4.831 ppm2

1.945

2.484 ppm2

4.972

3.422 ppm2

1.083

2.505 ppm2

;

6.173

1.596 ppm3

1.068

1.205 ppm2

1.900

3.031 ppm2

1.324

1.600 ppm2

1.333

1.547 ppm2

1.627

1.994 ppm2

A85 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	,	OR (	ASBI COR	5 6	1 188	40 48 C	WS T	New Or	85 85	88. 88. 99.	ASS ON CONTRACT	8
											مخرا	
			~		-	•	۰	•	3	•	<b>s</b>	
4.27			1.232	1.660	1.591	2.033	4.450	1.645	3.513	1.414	e.	
					_	_	_	_			~	
6.656 ppm2			2.141 ppm2	2.467 ppm2	3.866 ppm2	4.951 ppm2	0.740 ppm2	1.648 ppm2	1.056 ppm2	4.656 ppm2	3.177 ppm2	
4.656			2.14	2.4			9.7		1.05	4.65		
							_	!				
0.44566E+02 ppml	į		0.47549K+02 ppm1	0.12259E+03 ppml	0,387018+02 ppm1	0.31535E-03 ppm	0.36612E+02 ppml	ida C	0.56232K+02 ppml	0.103738+03 ppm1	0.10219E+03 ppm1	
66.03			19K+02	89E+0]	0.00	356.0	128+0	116.0	328.0	728.0	119E+0	
0.445666+02 ppm1			0.475	0.122	, se ,	0.315	9.366	0.192	0.562	0.103	6.103	
								0.100008-01 volume 0.192118-03 ppml	,	j	1 cme	
70 7			lo .	io fov	10 10	70 11		5	8	8	\$ . 0	
0.10000E.01 volume			0.10060E.01 volume	0.10000£.01 volume	0.10000E+01 volume	0.10000£+01 volume	0.10000E+01 volume	***************************************	0.100008+61 volume	0.10000E+01 volume	0.10000E-01 volume	
91.0			0.10	0.10	0.10							
HE JI	HB1 ))	HB1	HB2 )) HD14) We1ght HB2 ))	HB2 )) HG2V) weight HB2 ))	HK 1) H020) H 19ht	KD2V) KA )) Veight	HO1 )) HO2 )) HA2 ))	HA 1) HA 1) HEN 1 HEN 1	HDIV) HDIV) HBZ ))	H01) H01) H02) H02() Veight H02()	HD1() HD1() HB1 )) HB2 )) HB2 )) HB2 ))	KB2 ))
Deco very name HA name HB name				DAME HE				11 115	11 116	12742 K K K K K K K K K K K K K K K K K K K	DAME HE HE	•
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.468268.03 ppm1	0.21424E+03 ppm1	0.14748E.02 ppml	0.161528.03 ppm1	0.24679E-03 ppm1	0.346558+03 ppm3	0.59623K+03 ppm3	0.20695B+03 ppm1	0.97985E+02 ppm1	0,37936E+02 ppm1	0.29812K+02 ppm1	0.812698+02 ppm1	0.21510E+03 ppm1
.10000E-01 volume 0	0.10000K.01 volume 0	0.10000E.01 volume 0	0.10000E+01 volume 0	0.100066401 volume (	0.10000E+01 Volume	0.10000E+01 volume (	0.10000E+01 volume	0.10000K+01 VGlume	0.10000E+01 volume	0.10080E+81 volume	0.10900E.01 volume	0.10000E+01 volume
and name HG2%) sek 13242 weight 0 and name HB2 }}	neme HD21) 3322 weight name HD21) name HD21)	HD2() HB1 )) Weight HD2() HB ))	and name (G1%) and name (A )) sak 13392 weight G and name (G1%)	HD2() HB2()) W19hc HD2()	name HB1 )) name HB1 )) name HB4 ) name HB4 ) 13602 weight name HB4 ) name HB4 )	name HD30) name HB1 1) 3762 weight name HD30) name HB2 1)	name MD19) 1952 weight name HD19) name HD 19)	I name HBV ) I name HDIV) I4042 weight I name HBV ) I name HBV )	and name KD2) peck 14162 weight and name HB2) and name HB2)	115 11	and name HA )) and name HB2 )) sak 14202 weight and name HA )) and name HB1 ))	and name HD24) and name HB3 )) ak 14312 weight and name HD24)
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0.5e075E+02 ppm1	0.54622E.02 ppm1	0.20227E+03 ppm1	0.3080E-02 ppm1	0.84483E.02 ppm1	0.30551£+03 ppm1	0.526996+01 ppm1	0.336716.02 pm3	0.60076E+02 ppm1	34186E-02 ppm1	0.271088+03 ppm1	0.221586+02 ppm.1
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	4.459 ppm2	1.894 ppm2	2.980 ppm2	1.795 ppm2	1.796 ppm2	4.163 ppm2	0.760 ppm2	1.056 pps2	1.056 ppm2	1.036 ppm2	1.056 ppm2
	0.41948.02 ppm1	o sastageog ppm1	0.13879E+01 ppm1	0.608308:02 pm1	0.23532E+03 ppm1	0.37412E-02 ppm1 '	0.11144E.03 ppm1	0.780\$9E+02 ppml	O.BloshE+O2 ppm.	0.25206E+02 ppm1	0.89355E+02 ppm1
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and name KS }} and name KO1 }}		and name NG24) and name NG1 )) peek 21222 weight and name NG24) and name NB1 ))	and name HB )) 2 and name HD10) peak 21362 weight of and name HB )) end name HB2)	and name HGIs) and name HBis) peak 21432 weight o and name HGIIs)	and name HOIV) and name HBI )) ank 21442 waight and name HOIV) and name HB2 ))	and name (H2 )) and name (H2 )) and name (H2 )) ak 21502 weight and name (H2 )) and name (H2 ))	and name NG21) and name NA 1) peak 21552 weight o and name NG21) and name NA 1) and name NA 3)	HOIN)	name HOIN) 1592 Weight name HOIN) name HOIN)	MA 1) HB1 )) Weight	and name HGI1) peek 31639 weight o and name HGI1) and name HGI1) and name HGI1) and name HGI )
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0.34706E+02 ppm1	0.28161E+02 ppm1	0.152366+02 ppm1	0.16533E+02 ppm1	0.10950E+04 ppm1	0.387948+02 ppm1	0.12806E+04 ppm1	0.40558E+02 ppm1	0.24225E+02 ppm1	0.246915-03 ppm1	0.64481E-01 ppm1
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0.51512E+01 ppm1	0.33282E+02 ppm1	0.188765+02 ppm1	0.303716+02 ppm1	0.10851E+04 ppm1	0.20825E+02 ppm1	0.20830£+03 ppm1	0.44195E+02 ppml	0.61541E-02 ppm1	0.92579K•02 ppml	0.43784£+02 ppm1	0.821408+02 ppm1
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		0.21871K+02 ppm1		0.138728+02 psm1	:		0.28141E+02 pom1	:	0.147918+02 ppm1		0.11153E-03 ppm1	,		0.552966+03 ppml		0.103598+04 ppm1	:	0.51564E.03 ppm1		0.55730E+02 ppm1		0.18431E+03 ppm1			0.21924E+03 ppm1		
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and name KD% }	and name HE's and name RA	and name	and name HEN	6 and name HEN ) and name HDN ) peak 1763 weight	and name	and name	and name and name peak 1613	and name	and name HEN 1 and name HA 11 peak 1891 weight	and name HEN )	and name and name peak 2063	and name H23 1)	and name HZ3 )) and name HA ))	and name HEN ) and name HB )) peak 24 weight	and name	and name HDt } and name NA )) peak 94 weight	and name	and name HEV ) and name HG2 )) peak 104 weight	and name HDV )	and name HD1 ) and name HG12) ) peak 124 weight	and name	and name KD1 ) and name KD2 )) peak 114 weight	and name	and name HE1	Peak - 534		and name HA 1)
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\$.009 ppm3

4.213

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5.879

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1.791

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		7.666 ppm2	7.611 post			7.794 ppm3	L	7.794 ppm2		7.739 poes	•		7.739 ppm2	:	7.797 DOM2								
- 1	184 d	0.34056E+03 ppm1	0.19434E-03 ppm1			0.65395K+03 ppm1		0.27784E+03 ppm1		0.11824K+04 ppm1			0.46212E+03 ppm1		0.273408+03 pps1			0.206108.63		0 237016.03			
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	and name HD1 }} and name HD2 b and name HD2 b and name HD3 b and name HD4 } and name HD4 } and name HD3 }}	and name HET )	And name HE3 ))  And name HE3 1)  peak 1674 weight 0.10000E.01 volume 0.96896E.02 ppml 7.786 ppml  and name HE3 1)  and name HE3 1)	and name HER ) and name HER ) and name HER ) and name HER ) pash 1564 weight 0.10000E-01 volume 0.73775E-02 ppml 7.783 ppm2 and name HER )	and name KA and name KA and name KA and name HA	and names HUN ) and name HUN ) and name HUZ ) and name HUR ) and name HUR ) and name HUN )	and name HD1 and name HZ2 and name HZ2 and name HD1 and name HD1	peak 1704 weight 0.10000k:01 volume 0.312116:01 ppm1 7.787 ppm2 is and name RD1)  and name RE1)  and name RE1)  and name RE1)	peak 1734 weight 0.10000E-01 volume 0.7941EE-03 ppm1 7.779 ppm2 and name NDN )	and name HC1 ) peak 1734 weight 0.10000E-01 volume 0.1846E-03 ppm1 7.781 ppm2 and name HC3 )	and name HG 1) 2 and name HG1) 5 and name HG12) 6 and name HG12) Perek 1744 weight 0.100006.01 volume 0.934808.03 ppm1 7.781 ppm2
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lume 0.135878+03 ppm3	lume 0.17612E.01 ppm.1			volume 0.12754E:03 ppm1	lume 0.467288+02 ppm1	lume 0.63447E+03 ppm1 lume 0.23261E+03 ppm1 lume 0.11437E+03 ppm1	
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3.545	7.400	2.0.2	2.163	0.700 3.708	2.034	4	
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0.201355+01 ppm1	0.244915.03 ppm1	0.374248.03 ppm1	0.238586.03 ppm1	0.18782E+03 ppm1	0.12383E+03 ppm1	6.53166E-03 DEM1	
0.10000E+01 volume 0.10000E+01 volume	0.10000E-01 volume	0.10000£+01 volume 0.10000£+01 volume	0.10000E-01 volume	0.10000E+01 volume	0.10000E+01 volume 0.10000E+01 volume	0.10000E+01 vol.ume	
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7.005 ppm2

3.331

2.434

7.004 ppm2

1.494

7.005 ppm2

0.795

6.687 ppm2

0.796

5.740 ppm2

7.647

7.005 ppm2

4.636

7.005 ppm2

7.419

7.005 ppm2

1.249	7	4. 927	0.845 2.178		3.010	5. 255
7.005 ppm2	7.534 ppm2	7.689 ppm2	7.615 ppm2		7.616 ppm2	7.904 ppm2
0.77150E+02 ppm1	0.703412+03 ppm1	0.135328+03 ppm1	0.12437E:03 ppm1	·	0.140128.03 ppm.1	0.13962E-03 ppm1
0.10000E+01 volume 0.		0.10000E.01 volume 0.	0.10000E+01 volume 0.		0.10000E+01 volume 0.1	0.10000E+01 volume 0.1
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Table 4

## Hydrogen Bonding Restraints

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!Helix Z
assign (residue 19 and name HN ) (residue 15 and name O ) assign (residue 19 and name N ) (residue 15 and name O )
                                                                    1.80 0.0 0.40
                                                                    2.80 0.30 0.40
assign (residue 22 and name HN ) (residue 18 and name O)
                                                                    1.80 0.0 0.40
assign (residue 22 and name N
                                  ) (residue 18 and name O )
                                                                    2.80 0.30 0.40
assign (residue 23 and name HN ) (residue 19 and name 0 )
                                                                    1.80 0.0 0.40
assign (residue 23 and name N ) (residue 19 and name O)
                                                                    2.80 0.30 0.40
assign (residue 24 and name HN ) (residue 20 and name 0)
                                                                    1.80 0.0 0.40
assign (residue 24 and name N ) (residue 20 and name O)
                                                                    2.80 0.30 0.40
assign (residue 25 and name HN ) (residue 21 and name 0 )
                                                                    1.80 0.0 0.40
assign (residue 25 and name N
                                  ) (residue 21 and name O )
                                                                    2.80 0.30 0.40
!Helix B
assign (residue 75 and name HN ) (residue 71 and name 0 ) assign (residue 75 and name N ) (residue 71 and name 0 )
                                                                    1.80 0.0 0.40
                                                                    2.80 0.30 0.40
!assign (residue 77 and name HN ) (residue 73 and name O )
                                                                     1.80 0.0 0.40
!assign (residue 77 and name N ) (residue 73 and name O)
                                                                     2.80 0.30 0.40
assign (residue 78 and name HN ) (residue 74 and name 0 )
                                                                    1.80 0.0 0.40
assign (residue 78 and name N ) (residue 74 and name O)
                                                                    2.80 0.30 0.40
assign (residue 79 and name HN ) (residue 75 and name O)
                                                                    1.80 0.0 0.40
assign (residue 79 and name N \, ) (residue 75 \, and name O \,)
                                                                    2.80 0.30 0.40
!assign (residue 80 and name HN ) (residue 76 and name O )
                                                                     1.80 0.0 0.40
!assign (residue 80 and name N
                                  ) (residue 76 and name O )
                                                                     2.80 0.30 0.40
assign (residue 81 and name HN ) (residue 77 and name O)
                                                                    1.80 0.0 0.40
assign (residue 81 and name N ) (residue 77 and name O)
                                                                    2.80 0.30 0.40
assign (residue 82 and name HN ) (residue 78 and name O)
                                                                    1.80 0.0 0.40
assign (residue 82 and name N ) (residue 78 and name O)
                                                                    2.80 0.30 0.40
!Helix C
assign (residue 102 and name HN ) (residue 98 and name O )
                                                                    1.80 0.0 0.40
assign (residue 102 and name N ) (residue 98 and name O )
                                                                    2.80 0.30 0.40
assign (residue 103 and name HN ) (residue 99 and name O)
                                                                    1.80 0.0 0.40
assign (residue 103 and name N ) (residue 99 and name O)
                                                                    2.80 0.30 0.40
assign (residue 104 and name HN ) (residue 100 and name O ) assign (residue 104 and name N ) (residue 100 and name O )
                                                                     1.80 0.0 0.40
                                                                     2.80 0.30 0.40
assign (residue 105 and name HN ) (residue 101 and name O ) assign (residue 105 and name N ) (residue 101 and name O )
                                                                     1.80 0.0 0.40
                                                                     2.80 0.30 0.40
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1,000,000   1,000,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00	1,000,100,100,100,100,100,100,100,100,1	INICIAL FANC		Er 9690:	5.960359E+10R	Š					0.114	9
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1.00   0.00   Act NTPA   1   Att ACK   100   11.100     1.00   0.00   Act NTPA   1   Att ACK   100   11.100     1.00   0.00   Act NTPA   1   Att ACK   100   11.101     1.00   0.00   Act NTPA   1   Att ACK   100   11.101     1.00   0.00   Act NTPA   1   Att ACK   100   11.101     1.00   0.00   Act NTPA   1   Att ACK   100   11.101     1.00   0.00   Act NTPA   1   Att ACK   101   Att ACK   101     1.00   0.00   Act NTPA   1   Att ACK   1     1.00   0.00   Act ACK   Att ACK   1     1.00   0.00   Act ACK   Att ACK   1   Att ACK   1     1.00   0.00   Act ACK   Att ACK   1   Att ACK   1     1.00   0.00   Act ACK   Att ACK   1   Att ACK   1     1.00   0.00   Act ACK   Att ACK   1   Att ACK   1     1.00   0.00   Act ACK   A	1 100 0.00 Act Attach 1 101 Act 200 11.100 0.00 Act Attach 1 101 Act 200 11.100 0.00 Act Attach 1 101 Act 200 11.100 0.00 Act Attach 1 101 Act 200 11.101 0.00 Act Attach 1 101 Act 200 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201 11.101 0.00 Act Attach 1 10 101 HH 201	Dec-96 15:1	11.47	C1001	ed by user AT		-	×	200	7		•
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1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,	100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100		•		ACR ATOR	•			<b>:</b>	-13.586	12.034	۰
1, 10, 10, 10, 10, 10, 10, 10, 10, 10,	1.055 1.00 0.00 ACM ATTACK 11 10.01 HIZ 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11.01 11	1 127	•		ACE ATOM	• :	5 5		5 5	14.521	13.203	-
1. 155 1.00 0.00 Met Attor 11 075 11 11 11 11 11 11 11 11 11 11 11 11 11	100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100   100		• -		100	::			: :	779.77	13.068	-
	1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,		٠.		ACR ALUM	4:	2 :		3 3	-15.236	13.953	۰
1.177 1.00 0.00 Acid Attack 11 141 181 181 181 181 181 181 181 181	1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,		٠.		ACH ALL	3			5	-15.260	13.645	•
1, 10, 10, 10, 10, 10, 10, 10, 10, 10,	1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 Acid ATOM 15 612 M M 10 115.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 1 15.555 1.15 1.00 0.00 B M 10 ATOM 15 612 M M 10 ATOM 15	10.1.	•		ACH ATOM	2	191		<b>5</b>	- 14.591	13.045	•
2.056 1.00 0.00 Acti ATCH 15 GC 181 101 115.397 2.056 1.00 0.00 Acti ATCH 15 GC 181 117 101 117.392 2.056 1.00 0.00 Acti ATCH 15 GC 181 118 201 116.205 2.0778 1.00 0.00 Acti ATCH 15 GC 181 118 201 116.205 2.0778 1.00 0.00 Acti ATCH 20 CC 181 118 201 116.205 2.078 1.00 0.00 Acti ATCH 20 CC 181 118 201 119.302 2.087 1.00 0.00 Br ATCH 20 CC 187 11 11.323 2.087 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.323 2.091 1.00 0.00 Br ATCH 20 CC 187 11 17.333 2.091 1.00 0.00 Br A	1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00	5.940 -1.10	-		ACH ATOM	ž	HB2		<b>5</b>	-15.669	13.578	-
1.739 1.00 0.00 Acti ATUM 11 to 101 HIM 201 1.1332 1.057 1.00 0.00 Acti ATUM 11 to 101 HIM 201 1.1332 1.057 1.00 0.00 Acti ATUM 11 to 102 HIM 201 1.15.201 2.775 1.00 0.00 Acti ATUM 12 to 121 HIM 201 1.15.201 2.785 1.00 0.00 Acti ATUM 21 HIM 201 1.15.201 2.785 1.00 0.00 Acti ATUM 21 HIM 201 1.15.201 2.785 1.00 0.00 Acti ATUM 21 HIM 201 1.15.201 2.785 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.785 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 201 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM 21 HIM 21 1.15.201 2.781 1.00 0.00 Br ATUM 21 HIM	1.739 1.00 0.00 Act ATM ATM 15 MD1 HIN 201 1.7332 1.05 0.00 Act ATM 21 MD1 HIN 201 1.7332 1.05 0.00 Act ATM 21 MD1 HIN 201 1.7541 1.05 1.00 0.00 Act ATM 21 MD1 HIN 201 1.6460 1.7373 1.00 0.00 Act ATM 21 MD1 HIN 201 1.6261 1.7373 1.00 0.00 Act ATM 21 MD1 HIN 201 1.9230 1.737 1.00 0.00 Act ATM 22 Act ATM 21 MD1 HIN 201 1.9230 1.737 1.00 0.00 Bro ATM 22 Act ATM 22	5.009 -0.05	~		ACH ATOM	5	8		50	-16.397	14.412	
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1.55 1.00 0.00 0.00 Aci ATUN 12 MET HIN 101 1.15 1.00 0.00 Aci ATUN 12 MET HIN 101 1.15 1.00 0.00 Aci ATUN 12 MET HIN 101 1.10 0.00 0.00 BPD ATUN 12 MET HIN 101 1.10 0.00 BPD ATUN 12 MET HIN 12 MET HIN 101 1.10 0.00 BPD ATUN 12 MET HIN 11 1.10 0.00 BPD ATUN 12 MET HIN 11 1.10 0.00 BPD ATUN 12 MET HIN 12 MET HI	1.3.16	6.135 -2.72	1.00	00.0	ACTA ATOM	: 5	1 1 1 1 1		: 6	10 220	6.370	
1.1577   1.000   0.000   Mod Afront   1.1577	1.1577 1.00 0.00 NOT ACTA ATTOM 12 OF OLD	6.732			ACT ATOM	: :			: :	27.67	5.603	-
1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00	1,114   1,00   0,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00   1,00			9 6	ACT ATOM	: :			Ξ.	11.916	5.783	Ä
	1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00	2 6 6 6 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7		3	ACH ALCH	; ;	3 \ 5 •		٠	21.272	5.354	ä
1.111   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0	1,111   1,100   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00	٠,	• -			•		;	٠.	28.103	\$ .003	ä
	1,114   1,100   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00		٠.		200	: :	ξ,	;	٠.	20.00	6.79	÷
1,144   1,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00   0,00	1,144   1,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,000   0,00				1000	:	, ,	;	٠.	201.10	7.614	÷
1,111   1,100   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00					1000	:	, ,	;	٠.	77	1.173	÷
1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00	1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,000   1,00				100	: :		;;	٠.	20. 100	6.206	ń
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1.4660 1.000 0.000 BED ATCH 41 C SER 2 1.1565 1.000 0.000 BED ATCH 41 C SER 2 1.1565 1.000 0.000 BED ATCH 41 C SER 2 1.1565 1.000 0.000 BED ATCH 41 H H H H H H H H H H H H H H H H H H	1.446. 1.00 0.00 RED ATCH 41 C SER 2 1.146. 1.00 0.00 RED ATCH 41 C SER 2 1.146. 1.00 0.00 RED ATCH 41 H H H H H H H H H H H H H H H H H H	16.857 2.9	69 1.0	0.00	BrD ATOM	÷	2	98.B	~	26.478	6.206	7
4.236 1.00 0.00 BD A704 4.1 M M M M M M M M M M M M M M M M M M M	1.156 1.00 0.00 BED ATON 41 0 0.58 13 15 15 15 10 0.00 BED ATON 41 11 11 11 11 11 11 11 11 11 11 11 11	19.429 2.6	0.1	0.00	Brb Atom	Ŧ	Ü	Z 25	~	27.415	7.025	ř
1.155 1.00 0.00 BPD ATON 45 11 H H H H H H H H H H H H H H H H H H	1.155 1.00 0.00 BPD A7094 4.1 N H H H H H H H H H H H H H H H H H H	15.601 4.2	0.1		BrD ATOM	Ç	0	<b>3</b>	~	26.900	6.155	
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5.775 1.00 0.00 BED ATON 41 CB H18 13 14 15 15 10 0.00 BED ATON 45 H18 H18 13 14 15 15 10 0.00 BED ATON 45 H18 H18 13 15 15 15 15 15 15 15 15 15 15 15 15 15	5.775 1.00 0.00 BED ATCH 41 CE H H15 13 14 15 15 10 0.00 BED ATCH 42 H15 H15 13 14 15 15 15 10 0.00 BED ATCH 44 H15 H15 13 15 15 10 0.00 BED ATCH 45 H15 H15 13 15 15 15 15 15 15 15 15 15 15 15 15 15	14.624 6.3	142 1.0	0.00	Brb ATOM	÷	±	818	-	24.652	6.286	ō
7.179 1.00 0.00 BED ATON 48 BEB 118 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	7.179 1.00 0.00 BED ATON 48 MIN HIS 13 14 15 15 15 10 10 10 BED ATON 49 MIN HIS 13 15 15 15 15 15 15 15 15 15 15 15 15 15	13.972 5.7	175 1.0	۰	BrD ATOM	Ç	8	118	-	29.356	4.740	-
4.178 1.00 0.00 BED ATOM 64 BEB 115 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	4.178 1.00 0.00 BPD ATCH 44 BEB 115 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	15.176 7.3	199 1:0	_	BrD ATOM	;	HBI	118	^	29.337	4.570	7
6.339 1.00 0.00 BPD ATOM \$1 00 WHS 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	6.339 1.00 0.00 BPD ATOM \$1 00 M18 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	14.428 0.1	178 1.00	•	BrD ATOM	ŧ	H82	aie	-	30.333	1.617	-
9.025 1.00 0.00 BPD ATOM 51 MD1 HIS 3 3 9,445 1.00 0.00 BPD ATOM 51 MD1 HIS 3 3 9,445 1.00 0.00 BPD ATOM 53 MD1 HIS 3 3 9,445 1.00 0.00 BPD ATOM 54 MD2 HIS 3 10 10 10 10 10 10 10 10 10 10 10 10 10	9.025 1.00 0.00 BED ATON 51 MILES 3 1918 15 3 1946 25 1.00 0.00 BED ATON 51 MILES 3 1918 15 3 1946 25 1.00 0.00 BED ATON 51 MILES 3 1918 15 3 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25 1946 25	15.184 6.9	139 1.0	_	BrD ATOM	ŝ	8	418	~	29.137	1.529	٠
9-462 1.00 0.00 BPD ATON 53 HIN HIS 3 17.755 1.00 0.00 BPD ATON 53 HIN HIS 3 17.755 1.00 0.00 BPD ATON 54 HID HIS 3 17.755 1.00 0.00 BPD ATON 55 HIS 13 10.135 1.00 0.00 BPD ATON 55 HIS 13 10.135 1.00 0.00 BPD ATON 55 HIS 13 10.135 1.00 0.00 BPD ATON 55 HIS 118 3 10.135 1.00 0.00 BPD ATON 55 HIS 118 118 118 118 118 118 118 118 118 11	9.462 1.00 0.00 BED ATON 53 BIN HS 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	16.512 0.0	139 1.0	_	Bro Atom	3	ē	118	-	28.235	3.464	
7,755 1.00 0.00 BED ATON 53 CORN 18 3 3 7 7 5 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1.455 1.00 0.00 BED ATOM 53 COLD HIS 13 1.00 0.00 BED ATOM 54 HIZD HIS 13 1.00 0.00 BED ATOM 54 HIZD HIS 13 1.00 0.00 BED ATOM 55 CEL MIS 13 10.10 0.00 BED ATOM 55 HIS 11 13 10.15 1.00 0.00 BED ATOM 55 HIS 11 13 10.15 1.00 0.00 BED ATOM 56 HIS 13 10.20 0.00 BED ATOM 56 CEL HIS 13 10.20 0.00 BED ATOM 56 CEL HIS 13 10.20 0.00 BED ATOM 51 HI MET 4 5.555 1.00 0.00 BED ATOM 52 HIS 14 HIS 5.555 1.00 0.00 BED ATOM 52 HIS 14 HIS 5.555 1.00 0.00 BED ATOM 52 HIS 14 HIS 5.555 1.00 0.00 BED ATOM 52 HIS HIS 52 HIS	16.718 9.0	162 1.0	_	BrD ATOM	S	E	418	~	27.659		: ;
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BED ATON 55 REA BED ATON 60 0 BED ATON 61 K BED ATON 61 K BED ATON 62 KK	BITO ATOM 58 HEA BITO ATOM 60 0 BITO ATOM 61 N BITO ATOM 61 K BITO ATOM 61 CA BITO ATOM 64 KA	*****			1000		5			37. 00	7.0	÷
BED ATON 539 C BED ATON 60 0 BED ATON 61 N BED ATON 62 KN	BID ATON 539 C BID ATON 60 0 BID ATON 61 N BID ATON 62 KN BID ATON 64 KA		•	3 6	3 4		1,		٠.	20.10	4.055	÷
BrD ATCH 60 0 BrD ATCH 61 N BrD ATCH 62 KN	BrD ATCH 60 0 BrD ATCH 61 N BrD ATCH 62 KN BrD ATCH 64 CA	19.366	23	0.00	Bro Ares			116		26.991	2.048	ē
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